



## Final Program Guide

### To locate your presentation:

- Refer to the Oral Presenters or Poster Presenters list for your name and the page number where your presentation is listed.
- Locate the page in the program-by-day pages.

## Abstract Book

### To locate your abstract:

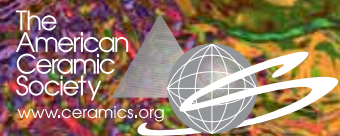
- Refer to the session topics in the front pages or the author index at the end of the pdf for the page number.
- Locate the page number and your abstract.



# CONFERENCE GUIDE

## 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING

MAY 22 – 26, 2022



HYATT REGENCY BALTIMORE | BALTIMORE, MARYLAND USA

<https://ceramics.org/gomd2022>



# ACERS *celebrates* the INTERNATIONAL YEAR OF GLASS

## National Day of Glass Conference

April 5-7, 2022 | Washington, DC

\*All speaker and panel recordings from this event are available at:  
[ceramics.org/ndog](http://ceramics.org/ndog)

## 2022 Glass and Optical Materials Division Annual Meeting (GOMD 2022)

May 22-26, 2022 | Baltimore, MD

[ceramics.org/gomd2022](http://ceramics.org/gomd2022)

## ACerS 124th Annual Meeting with Materials Science & Technology 2022 (MS&T22)

October 9-13, 2022 | Pittsburgh, PA

[ceramics.org/ms&t22](http://ceramics.org/ms&t22)

## welcome

### Dear Colleagues and Friends,

On behalf of The American Ceramic Society, welcome to the Glass & Optical Materials Division Meeting (GOMD 2022). We have over 250 oral and poster presentations that explore the fundamental nature of the glassy state, glass applications in healthcare, energy and environment, glass manufacturing challenges, nuclear waste immobilization, optical and optoelectronic materials, and more. GOMD2022 will provide a unique opportunity for glass scientists and technologists to interact.

GOMD2022 covers the latest advances in glass science and technology. Technical leaders from industry, national laboratories, and academia will lead four symposia and 20 technical session topics that provide an open forum for glass scientists and engineers from around the world to present and exchange findings on recent advances in various aspects related to glass science and technology. The poster session will highlight late-breaking research and feature the annual student poster contest.

Several special activities are planned in addition to the technical program:

- Renew acquaintances and get to know new faces within the GOMD community during the Welcome Reception on Sunday from 5:00 p.m. – 7:00 p.m.
- Special Award Lectures: The Stookey Lecture of Discovery Award (Monday morning), the George W. Morey Award (Tuesday morning), the Norbert J. Kreidl Award for Young Scholars and luncheon, sponsored by AGC (Tuesday at Noon), the Varshneya Frontiers of Glass Science lecture (Wednesday morning) and the Varshneya Frontiers of Glass Technology lecture (Thursday morning)
- Continue your learning experience by attending the Poster Session and Student Poster Competition on Monday from 6:30 p.m. – 8:30 p.m.
- Career Roundtable with panelists from industry, academia and government labs for undergraduates, graduates, postdoctoral researchers and young professionals on Wednesday from Noon to 1 p.m.
- GOMD attendees are invited to be our guests and continue networking with their colleagues during the conference banquet on Tuesday from 7:00 p.m. – 9:00 p.m. The L. David Pye Lifetime Achievement award will be presented by ACerS. *The Journal of Non Crystalline Solids* Mott award will be presented by Elsevier. The

winners

of the poster competition and Glorious Glass Demo competition will be announced.

**Special thanks to our sponsors AGC, Corning Incorporated, Guardian Glass, Owens-Corning, and Coe College.**

**The American Ceramic Society thanks you for participating in and being part of this year's meeting.**

## GOMD 2022 Program Chairs



**Ashutosh Goel,**  
Rutgers University



**Charmayne Lonergan**  
Pacific Northwest  
National Lab

## 2021-22 GOMD Officers

Chair: **Gang Chen**  
Ohio University

Chair-Elect: **Joseph Ryan**  
Pacific Northwest National  
Laboratory

Vice Chair: **Irene Peterson**  
Corning Research and Develop-  
ment Corporation

Secretary:  
**Michelle Korwin-Edson**  
Owens Corning

# 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING



<https://ceramics.org/gomd2022>

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## final program

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## WELCOME FROM THE AMERICAN CERAMIC SOCIETY (ACERS)

The ACerS community is open to all, and we're happy to have you with us. ACerS values diverse and inclusive participation within the field of ceramic science and engineering. We strive to promote involvement and access to leadership opportunity regardless of race, ethnicity, gender, religion, age, sexual orientation, nationality, disability, appearance, geographic location, career path or academic level.

If you are a new member or joining us for the first time, please see the events available in this program, or visit the ACerS registration desk to learn more.

For all guests, if you need access to a nursing mother's room or other special needs, please ask us at the ACerS registration desk. For childcare services, please check with the hotel concierge for a listing of licensed and bonded caregivers.

We hope you enjoy the conference and want you to know that all individuals are welcome at ACerS conferences and events.

# schedule-at-a-glance

## SUNDAY, MAY 22, 2022

Conference registration	4 – 6 p.m.	Constellation foyer (2nd floor)
Welcome reception	5 – 7 p.m.	Atrium (2nd floor)

## MONDAY, MAY 23, 2022

Conference registration	7 a.m. – 5:30 p.m.	Constellation foyer (2nd floor)
Stokey Lecture of Discovery (sponsored by Corning and Coe College)	8 – 9 a.m.	Constellation C/D (2nd floor)
Concurrent technical sessions	9:20 a.m. – 6 p.m.	2nd floor breakout rooms
Lunch on own	Noon – 1:30 p.m.	
Poster setup - students hang posters	2:30 – 5:30 p.m.	Atrium/Harborview (2nd floor)
Poster session and reception; student poster competition (sponsored by Corning)	6:30 – 8:30 p.m.	Atrium/Harborview (2nd floor)

## TUESDAY, MAY 24, 2022

Conference registration	7:30 a.m. – 5:30 p.m.	Constellation foyer (2nd floor)
George W. Morey Award lecture	8 – 9 a.m.	Constellation C/D (2nd floor)
Concurrent technical sessions	9:20 a.m. – 6 p.m.	2nd floor breakout rooms
Norbert J. Kreidl Award for Young Scholars (sponsored by AGC)	Noon – 1 p.m.	Constellation C/D (2nd floor)
Lunch on own	Noon – 1:30 p.m.	
GOMD general business meeting	5:45 – 6:45 p.m.	Constellation C/D (2nd floor)
Conference banquet	7 – 9 p.m.	Constellation A/B (2nd floor)

## WEDNESDAY, MAY 25, 2022

Conference registration	7:30 a.m. – 5 p.m.	Constellation foyer (2nd floor)
Varshneya Frontiers of Glass Science lecture	8 – 9 a.m.	Constellation C/D (2nd floor)
Concurrent technical sessions	9:20 a.m. – 6 p.m.	2nd floor breakout rooms
Student & Young Professionals Networking Panel	Noon – 1:20 p.m.	Constellation C/D (2nd floor)
Lunch on own	Noon – 1:30 p.m.	

## THURSDAY, MAY 26, 2022

Conference registration	7:30 a.m. – 3 p.m.	Constellation foyer (2nd floor)
Varshneya Frontiers of Glass Technology lecture	8 – 9 a.m.	Constellation C/D (2nd floor)
Concurrent technical sessions	9:20 a.m. – 12:40 p.m.	2nd floor breakout rooms

All live sessions will be recorded for registered attendees to view at the conclusion of the live conference. Available through the Bravura Connect O website until July 31, 2022.



# 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING



<https://ceramics.org/gomd2022>

## meeting regulations



No photography/recording

Cell phones silent



During oral sessions conducted during Society meetings, unauthorized photography, videotaping, and audio recording is strictly prohibited for two reasons: (1) conference presentations are the intellectual property of the presenting authors as such are protected, and (2) engaging in photography, videotaping, or audio recording is disruptive to the presenter and the audience. Failure to comply may result in the removal of the offender from the session or from the remainder of the meeting.

Note: The Society may engage photographers to photograph sessions for marketing and promotional purposes.

### MEETING REGULATIONS

The American Ceramic Society is a nonprofit scientific organization that facilitates the exchange of knowledge meetings and publication of papers for future reference. The Society owns and retains full right to control its publications and its meetings. The Society has an obligation to protect its members and meetings from intrusion by others who may wish to use the meetings for their own private promotion purpose. Literature found not to be in agreement with the Society's goals, in competition with Society services or of an offensive nature will not be displayed anywhere in the vicinity of the meeting. Promotional literature of any kind may not be displayed without the Society's permission and unless the Society provides tables for this purpose. Literature not conforming to this policy or displayed in other than designated areas will be disposed. The Society will not permit unauthorized scheduling of activities during its meeting by any person or group when those activities are conducted at its meeting place in interference with its programs and scheduled activities. The Society does not object to appropriate activities by others during its meetings if it is consulted with regard to time, place, and suitability. Any person or group wishing to conduct any activity at the time and location of the Society meeting must obtain permission from the Executive Director or Director of Meetings, giving full details regarding desired time, place and nature of activity.

**Diversity Statement:** The American Ceramic Society values diverse and inclusive participation within the field of ceramic science and engineering. ACerS strives to promote involvement and access to leadership opportunity regardless of race, ethnicity, gender, religion, age, sexual orientation, nationality, disability, appearance, geographic location, career path or academic level. Visit the registration desk if you need access to a nursing mother's room or need further assistance. For childcare services, please check with the concierge at individual hotels for a listing of licensed and bonded child care options. The American Ceramic Society plans to take photographs and video at the conference and reproduce them in educational, news

or promotional materials, whether in print, electronic or other media, including The American Ceramic Society's website. By participating in the conference, you grant The American Ceramic Society the right to use your name and photograph for such purposes. All postings become the property of The American Ceramic Society. During oral sessions conducted during Society meetings, unauthorized photography, videotaping and audio recording is prohibited. Failure to comply may result in the removal of the offender from the session or from the remainder of the meeting.

**Registration Requirements:** Attendance at any meeting of the Society shall be limited to duly registered persons.

**Disclaimer:** Statements of fact and opinion are the responsibility of the authors alone and do not imply an opinion on the part of the officers, staff or members of The American Ceramic Society. The American Ceramic Society assumes no responsibility for the statements and opinions advanced by the contributors to its publications or by the speakers at its programs; nor does The American Ceramic Society assume any liability for losses or injuries suffered by attendees at its meetings. Registered names and trademarks, etc. used in its publications, even without specific indications thereof, are not to be considered unprotected by the law. Mention of trade names of commercial products does not constitute endorsement or recommendations for use by the publishers, editors or authors.

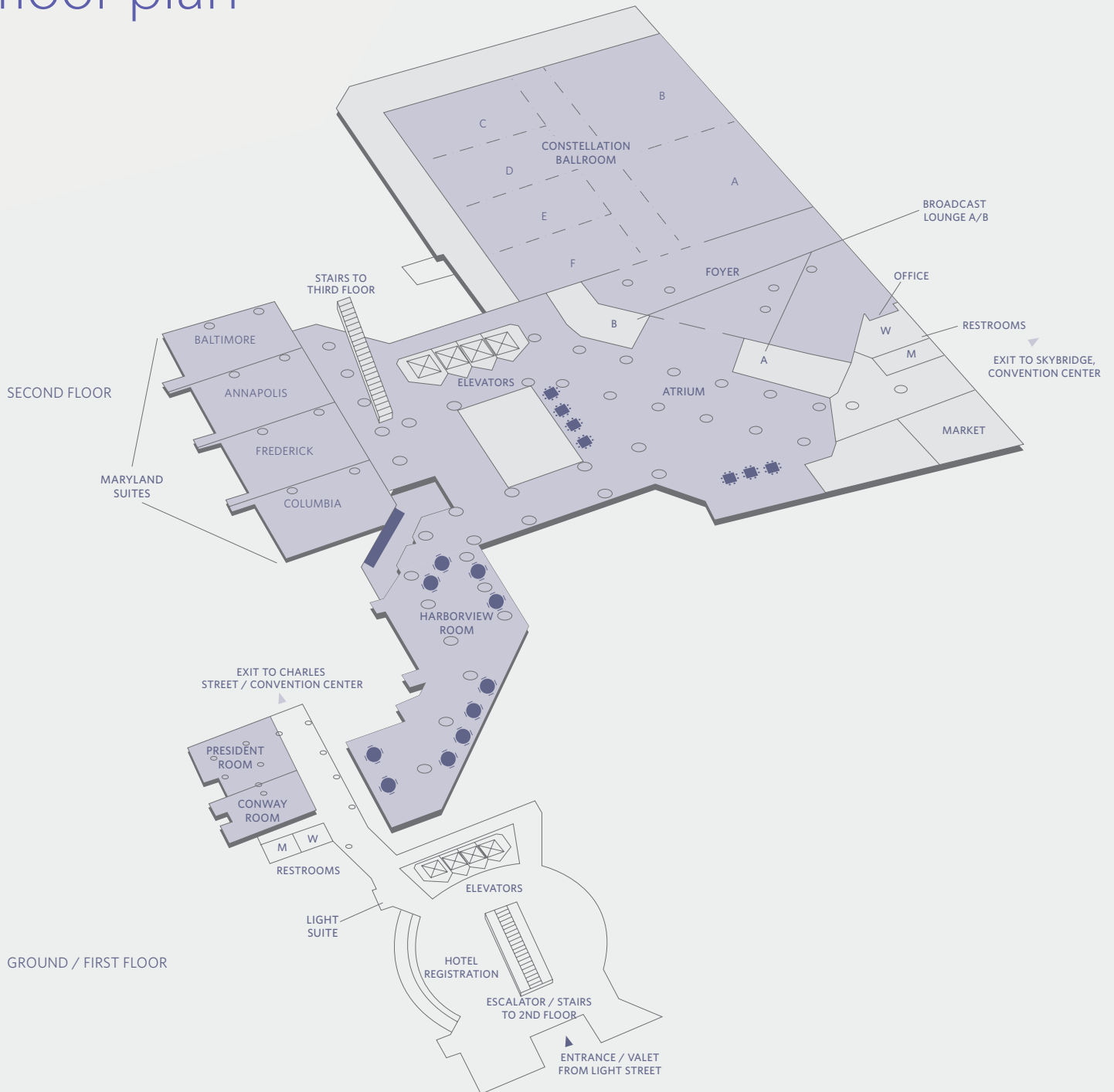
Final determination of the suitability of any information, procedure or products for use contemplated by any user, and the manner of that use, is the sole responsibility of the user. Expert advice should be obtained at all times when implementation is being considered, particularly where hazardous materials or processes are encountered.

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# floor plan





# 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING



<https://ceramics.org/gomd2022>

## award speakers

### Stookey Lecture of Discovery

Monday, May 23, 2022 | 8 – 9 a.m. | Constellation C/D



**Herbert Gleiter**, Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

Title: *Nanostructured glasses (Nano-glasses): The door to a new glass-based technology age: A glass age*

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### Varshneya Glass Science Lecture

Wednesday, May 25, 2022 | 8 – 9 a.m. | Constellation C/D



**Kathleen Richardson**, Pegasus Professor of Optics and Materials Science and Engineering and Florida Photonics Center of Excellence (FPCE) Professor at CREOL/ College of Optics and Photonics at the University of Central Florida, USA

Title: *Chalcogenide optical materials: A 'coming of age' story*

### George W. Morey Award Lecture

Tuesday, May 24, 2022 | 8 – 9 a.m. | Constellation C/D



**John Ballato**, Materials Science and Engineering, Clemson University, USA

Title: *Optical fiber meets the periodic table: The past, present, and future of the molten core method*

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### Varshneya Glass Technology Lecture

Thursday, May 26, 2022 | 8 – 9 a.m. | Constellation C/D



**Qiang Fu**, Senior Research Associate, Corning Incorporated, USA

Title: *From strong bioactive glasses to tough bio-inspired glass-ceramics: A journey towards damage-resistant materials*

### Norbert J. Kreidl Award for Young Scholars

Wednesday, May 25, 2022 | 12:15 – 1:05 PM | Constellation C/D



**Nagia Tagiara**, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Title: *Synthesis, structure and properties of pure TeO<sub>2</sub> glass, binary and ternary tellurite glasses*

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# 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING



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## sessions by symposium

SESSION TITLE	DATE	TIME	LOCATION
<b>AWARD LECTURES</b>			
Stookey Lecture of Discovery	May 23, 2022	8 - 9 AM	Constellation C/D (2nd floor)
George W. Morey Award Lecture	May 24, 2022	8 - 9 AM	Constellation C/D (2nd floor)
Norbert J. Kreidl Award for Young Scholars	May 24, 2022	12:15 - 1:15 PM	Constellation C/D (2nd floor)
Varshneya Glass Science Lecture	May 25, 2022	8 - 9 AM	Constellation C/D (2nd floor)
Varshneya Glass Technology Lecture	May 26, 2022	8 - 9 AM	Constellation C/D (2nd floor)
<b>POSTERS</b>			
Poster Session	May 23, 2022	6:30 - 8:30 PM	Atrium/Harborview (2nd floor)
<b>S1: FUNDAMENTALS OF THE GLASSY STATE</b>			
Mechanical Properties of Glasses: Indentation Responses	May 23, 2022	9:20 AM - 12 PM	Frederick (2nd floor)
Mechanical Properties of Glasses: Fracture and Crack Propagation	May 23, 2022	1:20 - 4:40 PM	Frederick (2nd floor)
Structure of Glasses I	May 24, 2022	9:20 - 11:10 AM	Columbia (2nd floor)
Structure of Glasses II	May 24, 2022	1:20 - 3:30 PM	Columbia (2nd floor)
Structure of Glasses III	May 24, 2022	3:40 - 5:10 PM	Columbia (2nd floor)
Topology and Rigidity	May 24, 2022	9:20 AM - 12:30 PM	Constellation E (2nd floor)
Glass Formation and Structural Relaxation I	May 24, 2022	1:20 - 3:40 PM	Constellation E (2nd floor)
Glass Formation and Structural Relaxation II	May 24, 2022	3:40 - 5:20 PM	Constellation E (2nd floor)
Improved Methods for Glass Structure Determination	May 25, 2022	9:20 AM - 12:10 PM	Constellation F (2nd floor)
Non-oxide Glasses and Glass-ceramics I	May 25, 2022	9:20 - 11:30 AM	Constellation E (2nd floor)
Non-oxide Glasses and Glass-ceramics II	May 25, 2022	1:20 - 3:20 PM	Constellation E (2nd floor)
Data-based Modeling and Machine Learning for Glass Science I	May 25, 2022	1:20 - 3:40 PM	Constellation C/D (2nd floor)
Data-based Modeling and Machine Learning for Glass Science II	May 25, 2022	3:40 - 5:40 PM	Constellation C/D (2nd floor)
Glass Crystallization and Glass Ceramics	May 25, 2022	1:20 - 5:20 PM	Frederick (2nd floor)
Predicting Glass Properties	May 25, 2022	1:20 - 3:20 PM	Constellation F (2nd floor)



SESSION TITLE	DATE	TIME	LOCATION
<b>S2: GLASS AND INTERACTIONS WITH ITS ENVIRONMENT: FUNDAMENTALS AND APPLICATIONS</b>			
Dissolution and Interfacial Reactions I: Dissolution behavior as a Function of Glass Composition	May 23, 2022	9:20 - 11:50 AM	Constellation C/D (2nd floor)
Dissolution and Interfacial Reactions II: Long-term Corrosion and Nuclear Waste Glasses	May 23, 2022	1:20 - 5:20 PM	Constellation C/D (2nd floor)
Dissolution and Interfacial Reactions III: Modeling Glass Dissolution and Glass Interaction with Various Environments	May 24, 2022	9:20 - 11:50 AM	Constellation C/D (2nd floor)
Glasses and Glass-ceramics for Healthcare	May 23, 2022	9:20 AM - 12 PM	Columbia (2nd floor)
Nuclear Waste Immobilization I	May 24, 2022	9:20 AM - 12:10 PM	Frederick (2nd floor)
Nuclear Waste Immobilization II	May 24, 2022	1:20 - 5 PM	Frederick (2nd floor)
Surfaces and Coatings	May 26, 2022	9:20 AM - 12:40 PM	Constellation F (2nd floor)
<b>S3: OPTICAL AND ELECTRONIC MATERIALS AND DEVICES: FUNDAMENTALS AND APPLICATIONS</b>			
Optical and Photonic Glasses and Glass-ceramics I	May 23, 2022	9:20 - 11:30 AM	Constellation E ((2nd floor)
Optical and Photonic Glasses and Glass-ceramics II	May 23, 2022	1:20 - 3:30 PM	Constellation E (2nd floor)
Glass-based Photonics I: Bulk and Fiber Devices	May 23, 2022	1:20 - 3:20 PM	Columbia (2nd floor)
Glass-based Photonics II: Planar Devices	May 23, 2022	3:20 - 4:50 PM	Columbia (2nd floor)
Charge and Energy Transport in Disordered Materials	May 24, 2022	1:20 - 4:20 PM	Constellation F (2nd floor)
Laser Interactions with Glasses	May 25, 2022	9:20 AM - 12:10 PM	Frederick (2nd floor)
Optical Fibers and Waveguides	May 26, 2022	9:20 - 11 AM	Frederick (2nd floor)
<b>S4: GLASS TECHNOLOGY AND CROSS-CUTTING TOPICS</b>			
Green Manufacturing	May 23, 2022	9:20 - 11:40 AM	Constellation F (2nd floor)
Forming and Coatings	May 23, 2022	1:20 - 3:10 PM	Constellation F (2nd floor)
Glass Challenges	May 23, 2022	3:40 - 4:40 PM	Constellation F (2nd floor)
Batch to Glass Conversion	May 24, 2022	9:20 AM - 12 PM	Constellation F (2nd floor)
Sol-gel Processing of Glasses and Ceramic Materials	May 25, 2022	9:20 - 11:50 AM	Columbia (2nd floor)
3D Printing of Glass	May 25, 2022	1:20 - 4:20 PM	Columbia (2nd floor)

# 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING



<https://ceramics.org/gomd2022>

## student events

### Meet the Editor of ACerS

*International Journal of Applied Glass Science*



**Mario Affatigato**, Editor of *IJAGS*, will be available at the following times:

**Monday, May 23** at the poster session 6:30-7:30 p.m.

In the Constellation Foyer near registration at break times:

**Tuesday, May 24** 9-9:20 a.m.  
3:20-3:40 p.m.

**Wednesday, May 25** 9-9:20 a.m.

### Student Poster Competition

Monday, May 23 | 6:30 – 8:30 p.m.

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This year's student competition will take place on Monday evening as part of the regular poster session from 6:30 – 8:30 p.m. on the second floor Atrium level of the hotel. This year's contest is organized by Charmayne Lonergan of Pacific Northwest National Laboratories.

**Poster setup is Monday from Noon - 4 p.m.**

Winners announced at conference dinner on Tuesday.



### Student & Young Professional Networking Career Panel Luncheon

Wednesday, May 25 | Noon – 1:20 p.m. | Room: Constellation C/D

Students, post-docs, and young professionals are invited to a networking luncheon that will include panelists representing industry, government, and academia. This is an opportunity to ask questions of professionals in a casual environment on a number of diverse topics (work-life balance, career opportunities, etc.).

The career professionals will rotate among attendees so that there will be an opportunity for candid discussions during the event. A complimentary lunch will be served. Pre-registration required - space is limited to the first 40 registrants.

#### PANELISTS:

- **Charmayne Lonergan**,  
Pacific Northwest National Laboratory (PNNL)
- **Ashutosh Goel**,  
Rutgers University
- **Nick Smith**,  
Corning Incorporated
- **Jincheng Du**, University of North Texas
- **Stephen Wilke**,  
Materials Development, Inc.

## symposium organizers

**Program Chairs:** **Ashutosh Goel**, Rutgers University  
**Charmayne Lonergan**, Pacific Northwest National Lab

### S1: FUNDAMENTALS OF THE GLASSY STATE

#### Session 1: Glass formation and structural relaxation

ORGANIZERS:

**Ozgur Gulbiten**, Corning Inc., USA  
**Sabyasachi Sen**, University of California Davis, USA  
**Collin Wilkinson**, GlassWRX, USA

#### Session 2: Glass Crystallization and Glass Ceramics

ORGANIZERS:

**Edgar Zanutto**, Federal University of Sao Carlos, Brazil  
**Matthew McKenzie**, Corning Inc., USA  
**Kisa Ranasinghe**, Kennesaw State University, USA

#### Session 3: Structural Characterizations of Glasses

ORGANIZERS:

**Daniel Neuville**, CNRS-IPGP-UP, France  
**Thibault Charpentier**, CEA Saclay, France  
**Oliver Alderman**, ISIS Neutron and Muon Source, UK

#### Session 4: Topology and Rigidity

ORGANIZERS:

**N.M. Anoop Krishan**, Indian Institute of Technology Delhi, India  
**Mathieu Bauchy**, University of California Los Angeles, USA  
**Morten Smedskjaer**, Aalborg University, Aalborg, Denmark

#### Session 5: Atomistic Simulation and Predictive Modeling of Glasses

ORGANIZERS:

**Sushmit Goyal**, Corning Inc., USA  
**Alfonso Pedone**, University of Modena and Reggio Emilia, Italy

#### Session 6: Data-based Modeling and Machine Learning for Glass Science

ORGANIZERS:

**Adama Tandia**, Corning Inc., USA  
**Aditya Kumar**, Missouri S&T, USA  
**Daniel Cassar**, Brazilian Center for Research in Energy and Materials, Brazil

#### Session 7: Mechanical Properties of Glasses

ORGANIZERS:

**Satoshi Yoshida**, AGC Inc., Japan  
**Timothy Gross**, Corning Inc., USA

#### Session 8: Non-Oxide Glasses and Glass-Ceramics

ORGANIZERS:

**Francisco Munoz**, CSIC-ICV, Spain  
**Pierre Lucas**, The University of Arizona, USA  
**Catherine Boussard-Pledel**, Institut des Sciences Chimiques de Rennes, France

#### Session 9: Glass under Extreme Conditions

ORGANIZERS:

**Dominique de Ligny**, FAU Erlangen-Nürnberg, Erlangen, Germany  
**Anindya Ghoshal**, Army Research Laboratory, USA  
**Anamul Haq Mir**, University of Huddersfield, UK



# 2022 GLASS & OPTICAL MATERIALS DIVISION ANNUAL MEETING



<https://ceramics.org/gomd2022>

## symposium organizers

### **S2: GLASS AND INTERACTIONS WITH ITS ENVIRONMENT — FUNDAMENTALS AND APPLICATIONS**

#### **Session 1: Glasses and Glass-ceramics for Healthcare**

ORGANIZERS:

**Hrishikesh Kamat**, Glidewell Dental Laboratories, USA  
**Delia Brauer**, University of Jena, Germany  
**Saurabh Kapoor**, Sterlite Technologies Ltd., India

#### **Session 2: Nuclear Waste Immobilization**

ORGANIZERS:

**Sophie Schuller**, CEA Marcoule, France  
**Kai Xu**, Wuhan University of Technology, China  
**Michael Ojovan**, The University of Sheffield, UK

#### **Session 3: Dissolution and Interfacial Reactions**

ORGANIZERS:

**Nicholas Stone-Weiss**, Corning Inc., USA  
**Stephane Gin**, CEA Marcoule, France  
**Jincheng Du**, University of North Texas, USA

#### **Session 4: Surfaces and Coatings**

ORGANIZERS:

**Matthew Linford**, Bingham Young University, USA  
**Joy Banerjee**, Corning Inc., USA  
**Adam Polcyn**, Vitro Architectural Glass, USA

### **S3: OPTICAL AND ELECTRONIC MATERIALS AND DEVICES — FUNDAMENTALS AND APPLICATIONS**

#### **Session 1: Laser Interactions with Glasses**

ORGANIZERS:

**Casey Schwarz**, Ursinus College, USA  
**Keith J. Veenhuizen**, Lebanon Valley College, USA

#### **Session 2: Charge and Energy Transport in Disordered Materials**

ORGANIZER:

**Caio Bragatto**, Coe College, USA

#### **Session 3: Optical Fibers and Waveguides**

ORGANIZERS:

**Jiawei Luo**, OFS Laboratories, USA  
**Sylvain Danto**, ICMCB, University of Bordeaux, France  
**Saurabh Kapoor**, Sterlite Technologies Ltd., India

#### **Session 4: Glass-based Optical Devices and Detector Applications**

ORGANIZERS:

**Juejun Hu**, Massachusetts Institute of Technology, USA  
**Hongtao Lin**, Zhejiang University, China  
**Badri Gomatam**, Sterlite Technologies Ltd., India

#### **Session 5: Optical and Photonic Glasses and Glass-Ceramics**

ORGANIZER:

**Laetitia Petit**, Tampere University, Finland

### **S4: GLASS TECHNOLOGY AND CROSS-CUTTING TOPICS**

#### **Session 1: Sol-gel Processing of Glasses and Ceramic Materials**

ORGANIZERS:

**Lisa Klein**, Rutgers University, USA  
**John Kieffer**, University of Michigan, USA

#### **Session 2: Challenges in Glass Manufacturing**

ORGANIZER:

**Irene Peterson**, Corning Inc., USA

#### **Session 3: 3D-printing of Glass**

ORGANIZERS:

**SK Sundaram**, Alfred University, USA  
**Qiu Jianrong**, Zhejiang University, China

## Oral Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
<b>A</b>					<b>H</b>				
Agnello, G.	26-May	11:20AM	Constellation F (Second floor)	18	Han, T.	25-May	2:20PM	Constellation C/D (Second floor)	16
Alderman, O.L.	24-May	4:50PM	Columbia (Second floor)	13	Hardin, T.J.	24-May	9:20AM	Constellation E (Second floor)	10
Almutairi, B.S.	24-May	9:50AM	Constellation E (Second floor)	10	Harrison, M.T.	23-May	2:10PM	Constellation C/D (Second floor)	6
Alvarez, R.	23-May	1:50PM	Constellation E (Second floor)	7	Hausmann, B.D.	24-May	11:30AM	Constellation C/D (Second floor)	11
Ammu, P.	25-May	10:50AM	Constellation F (Second floor)	14	Hossain, Z.	23-May	11:40AM	Frederick (Second floor)	4
Ammu, P.	25-May	5:00PM	Constellation C/D (Second floor)	16	Hu, J.	23-May	3:50PM	Columbia (Second floor)	7
Amoroso, J.	24-May	4:00PM	Frederick (Second floor)	14	Huang, L.	25-May	1:50PM	Constellation F (Second floor)	17
<b>B</b>					<b>I</b>				
Balasubramanya, N.	24-May	1:40PM	Frederick (Second floor)	13	Icenhower, J.P.	23-May	10:30AM	Constellation C/D (Second floor)	4
Balasubramanya, N.	24-May	2:00PM	Frederick (Second floor)	13	Inagaki, Y.	23-May	2:50PM	Constellation C/D (Second floor)	6
Ballato, J.	24-May	8:10AM	Constellation E (Second floor)	10	Ispas, S.	25-May	1:20PM	Constellation F (Second floor)	17
Barker, C.	25-May	11:50AM	Frederick (Second floor)	15	<b>J</b>				
Bauchy, M.	24-May	12:10PM	Constellation E (Second floor)	10	Jain, H.	25-May	1:20PM	Frederick (Second floor)	16
Bauchy, M.	25-May	10:10AM	Constellation F (Second floor)	14	Jan, A.	23-May	5:00PM	Constellation C/D (Second floor)	7
Bauchy, M.	25-May	1:50PM	Constellation C/D (Second floor)	16	Jan, A.	25-May	11:50AM	Constellation F (Second floor)	15
Beg, M.C.	24-May	5:00PM	Constellation E (Second floor)	12	Jarvis, S.M.	24-May	11:20AM	Constellation F (Second floor)	12
Bellafatto, A.J.	23-May	11:20AM	Frederick (Second floor)	4	Jia, R.	24-May	3:00PM	Frederick (Second floor)	13
Bellows, C.	23-May	2:10PM	Constellation E (Second floor)	7	Jitianu, A.	25-May	11:10AM	Columbia (Second floor)	16
Bennett, T.	25-May	9:20AM	Constellation E (Second floor)	15	Jubera, V.	23-May	9:20AM	Constellation E (Second floor)	5
Bertani, M.	25-May	10:30AM	Constellation F (Second floor)	14	<b>K</b>				
Bhattoo, R.	25-May	3:40PM	Constellation C/D (Second floor)	16	Kamat, H.	24-May	10:30AM	Columbia (Second floor)	10
Bhattoo, R.	25-May	5:20PM	Constellation C/D (Second floor)	16	Kang, M.	25-May	10:20AM	Frederick (Second floor)	15
Bishnoi, S.	25-May	4:40PM	Constellation C/D (Second floor)	16	Kaspar, T.	26-May	10:30AM	Constellation F (Second floor)	18
Blanc, W.	26-May	9:20AM	Frederick (Second floor)	19	Kassab, L.R.	23-May	1:20PM	Constellation E (Second floor)	7
Blatt, R.L.	23-May	11:10AM	Constellation C/D (Second floor)	4	Kelton, K.F.	25-May	3:30PM	Frederick (Second floor)	17
Braga, M.	24-May	1:20PM	Constellation F (Second floor)	14	Kerisit, S.N.	23-May	3:30PM	Constellation C/D (Second floor)	6
Budziszewski, C.	26-May	12:00PM	Constellation F (Second floor)	19	Keshri, S.R.	23-May	11:00AM	Columbia (Second floor)	5
<b>C</b>					<b>L</b>				
Calahoo, C.	23-May	10:10AM	Constellation C/D (Second floor)	4	Lallukka, M.S.	23-May	10:10AM	Columbia (Second floor)	5
Casalena, L.	23-May	2:30PM	Constellation E (Second floor)	7	Le Coq, D.	25-May	1:20PM	Constellation E (Second floor)	17
Caurant, D.	24-May	9:50AM	Columbia (Second floor)	10	Lee, H.	23-May	10:00AM	Frederick (Second floor)	4
Charpentier, T.	25-May	9:50AM	Constellation F (Second floor)	14	Lee, H.	24-May	2:40PM	Constellation E (Second floor)	12
Charpentier, T.	25-May	1:20PM	Constellation C/D (Second floor)	16	Leonard, R.L.	23-May	9:50AM	Constellation E (Second floor)	5
<b>D</b>					<b>M</b>				
Damodaran, K.	23-May	9:50AM	Constellation C/D (Second floor)	4	Macrelli, G.	23-May	3:30PM	Frederick (Second floor)	6
DeCeanne, A.V.	25-May	4:20PM	Frederick (Second floor)	17	Maehara, T.	23-May	10:50AM	Constellation F (Second floor)	6
Delaye, J.	23-May	4:40PM	Constellation C/D (Second floor)	7	Mahadevan, T.S.	24-May	9:20AM	Constellation C/D (Second floor)	11
DeMaere, P.N.	24-May	11:40AM	Constellation F (Second floor)	12	Malek, J.	24-May	4:10PM	Constellation E (Second floor)	12
Destino, J.F.	25-May	9:50AM	Columbia (Second floor)	15	Mansfield, J.T.	24-May	4:20PM	Frederick (Second floor)	14
Dierolf, V.	25-May	9:20AM	Frederick (Second floor)	15	Marcial, J.	24-May	9:20AM	Constellation F (Second floor)	12
Ding, L.	23-May	11:00AM	Frederick (Second floor)	4	Marcial, J.	24-May	3:40PM	Frederick (Second floor)	14
Dong, Y.	24-May	11:30AM	Frederick (Second floor)	11	Martin, M.P.	25-May	3:00PM	Constellation E (Second floor)	17
Drnovsek, N.	24-May	10:50AM	Constellation C/D (Second floor)	11	Matsubara, R.	23-May	4:20PM	Constellation C/D (Second floor)	7
Du, J.	24-May	9:50AM	Constellation C/D (Second floor)	11	McCloy, J.	24-May	2:10PM	Columbia (Second floor)	13
Duval, A.	25-May	2:40PM	Constellation E (Second floor)	17	Mecholsky, J.	23-May	2:50PM	Frederick (Second floor)	6
<b>E</b>					<b>N</b>				
El Dib, G.	26-May	10:20AM	Frederick (Second floor)	19	Moghimi, L.	25-May	9:50AM	Constellation E (Second floor)	15
<b>F</b>					<b>O</b>				
Fang, G.	24-May	4:40PM	Frederick (Second floor)	14	<b>P</b>				
Fayon, F.	24-May	9:20AM	Columbia (Second floor)	10	<b>Q</b>				
Ferkl, P.	24-May	9:50AM	Constellation F (Second floor)	12	<b>R</b>				
Ferreira, E.B.	25-May	2:10PM	Frederick (Second floor)	16	<b>S</b>				
Floyd, A.	23-May	10:30AM	Constellation E (Second floor)	5	<b>T</b>				
Fry, A.L.	23-May	10:20AM	Frederick (Second floor)	4	<b>U</b>				
Fu, Q.	26-May	8:10AM	Constellation C/D (Second floor)	18	<b>V</b>				
<b>G</b>					<b>W</b>				
Gallais, L.	25-May	2:20PM	Columbia (Second floor)	18	<b>X</b>				
Ghardi, E.	23-May	2:50PM	Constellation E (Second floor)	8	<b>Y</b>				
Gin, S.	23-May	2:30PM	Constellation C/D (Second floor)	6	<b>Z</b>				
Gleiter, H.	23-May	8:10AM	Constellation C/D (Second floor)	4	<b>AA</b>				
Golovchak, R.	24-May	3:40PM	Constellation E (Second floor)	12	<b>AB</b>				
Grodsky, R.	24-May	11:10AM	Constellation C/D (Second floor)	11	<b>AC</b>				
Grunwald, T.	23-May	2:30PM	Constellation F (Second floor)	8	<b>AD</b>				
Guo, X.	23-May	1:20PM	Constellation C/D (Second floor)	6	<b>AE</b>				

# Presenting Author List

## Oral Presenters

Name	Date	Time	Room	Page Number	Name	Date	Time	Room	Page Number
Möncke, D.	23-May	4:00PM	Constellation F (Second floor)	8	Sørensen, S.S.	24-May	2:50PM	Constellation F (Second floor)	14
Möncke, D.	24-May	1:20PM	Columbia (Second floor)	13	Sorin, F.	26-May	9:50AM	Frederick (Second floor)	19
Moore, E.	23-May	9:50AM	Columbia (Second floor)	5	Spirrett, F.	25-May	2:50PM	Columbia (Second floor)	18
Moore, L.	25-May	5:00PM	Frederick (Second floor)	17	Stone-Weiss, N.	23-May	9:40AM	Frederick (Second floor)	4
Muijsenberg, E.H.	23-May	10:20AM	Constellation F (Second floor)	6	Strobl, C.	23-May	2:10PM	Constellation F (Second floor)	8
Müller, C.	25-May	10:20AM	Constellation E (Second floor)	15	Strong, K.T.	25-May	4:00PM	Frederick (Second floor)	17
Muller, I.S.	24-May	10:10AM	Constellation C/D (Second floor)	11	Sun, W.	25-May	11:30AM	Constellation F (Second floor)	15
Munoz, F.	25-May	4:20PM	Constellation E (Second floor)	17	Sundaram, S.K.	23-May	3:40PM	Constellation F (Second floor)	8
Musterman, E.J.	25-May	11:10AM	Frederick (Second floor)	15	Suratwala, T.I.	23-May	2:40PM	Columbia (Second floor)	7
Musterman, E.J.	25-May	2:30PM	Frederick (Second floor)	17	Swiler, D.R.	24-May	10:20AM	Constellation F (Second floor)	12
Myers, A.J.	23-May	11:20AM	Constellation F (Second floor)	6					
		<b>N</b>							
Nazhat, S.N.	23-May	10:30AM	Columbia (Second floor)	5	Tagiara, N.	24-May	12:25PM	Constellation C/D (Second floor)	12
Neeway, J.	23-May	1:50PM	Constellation C/D (Second floor)	6	Tang, M.	24-May	11:10AM	Frederick (Second floor)	11
Neeway, J.	23-May	4:00PM	Constellation C/D (Second floor)	7	Torres, V.M.	24-May	2:30PM	Constellation F (Second floor)	14
Neuville, D.R.	24-May	2:50PM	Columbia (Second floor)	13	Tostanoski, N.	25-May	10:50AM	Frederick (Second floor)	15
Niu, C.	24-May	10:50AM	Frederick (Second floor)	11	Troles, J.	25-May	3:50PM	Columbia (Second floor)	18
		<b>O</b>							
Ogrinc, A.L.	26-May	10:10AM	Constellation F (Second floor)	18	Urata, S.	25-May	2:50PM	Constellation F (Second floor)	17
Ohara, K.	24-May	3:40PM	Columbia (Second floor)	13					
Onodera, Y.	24-May	10:50AM	Constellation E (Second floor)	10	Veenhuizen, K.J.	25-May	11:30AM	Frederick (Second floor)	15
Ori, G.	25-May	9:20AM	Constellation F (Second floor)	14	Verger, L.	25-May	11:10AM	Constellation E (Second floor)	15
Otsuka, T.	23-May	10:50AM	Constellation E (Second floor)	5	Verheijen, O.	23-May	9:50AM	Constellation F (Second floor)	5
		<b>P</b>			Verné, E.	23-May	9:20AM	Columbia (Second floor)	5
Park, H.	25-May	2:10PM	Constellation F (Second floor)	17	Vogel, P.	23-May	1:50PM	Constellation F (Second floor)	8
Pedone, A.	25-May	4:40PM	Frederick (Second floor)	17	Vu, A.	25-May	2:40PM	Constellation C/D (Second floor)	16
Peterson, I.	25-May	1:50PM	Frederick (Second floor)	16					
Petit, L.	23-May	1:50PM	Columbia (Second floor)	7	Wang, G.	25-May	10:50AM	Columbia (Second floor)	16
Piatti, E.	23-May	11:20AM	Columbia (Second floor)	5	Weaver, J.L.	24-May	1:50PM	Constellation F (Second floor)	14
Pokorny, R.	24-May	9:20AM	Frederick (Second floor)	11	Weber, R.	24-May	4:30PM	Columbia (Second floor)	13
Popescu, C.	23-May	4:10PM	Columbia (Second floor)	7	Weyrauch, N.	23-May	1:50PM	Frederick (Second floor)	6
Poumellec, B.	25-May	9:50AM	Frederick (Second floor)	15	Wheaton, J.	24-May	2:10PM	Constellation F (Second floor)	14
Prasai, K.	25-May	11:10AM	Constellation F (Second floor)	14	Wilke, S.K.	24-May	10:50AM	Columbia (Second floor)	10
		<b>Q</b>			Wilkinson, C.	24-May	4:40PM	Constellation E (Second floor)	12
Qi, L.	25-May	3:30PM	Columbia (Second floor)	18					
Qin, Q.	23-May	10:50AM	Constellation C/D (Second floor)	4	Xu, X.	24-May	10:30AM	Frederick (Second floor)	11
Qin, Q.	24-May	10:30AM	Constellation C/D (Second floor)	11	Xu, X.	24-May	11:50AM	Frederick (Second floor)	11
		<b>R</b>							
Ranasinghe, K.S.	23-May	11:40AM	Columbia (Second floor)	5	Yadav, A.	23-May	10:40AM	Frederick (Second floor)	4
Reux, V.	25-May	10:50AM	Constellation E (Second floor)	15	Yeo, T.	24-May	2:20PM	Constellation E (Second floor)	12
Richardson, K.A.	25-May	8:10AM	Constellation C/D (Second floor)	14	Yuan, B.	24-May	4:10PM	Columbia (Second floor)	13
Richert, R.	24-May	1:20PM	Constellation E (Second floor)	12					
Rimsza, J.M.	23-May	1:20PM	Frederick (Second floor)	6	Zaki, M.	25-May	3:00PM	Constellation C/D (Second floor)	16
Ross, C.P.	23-May	9:20AM	Constellation F (Second floor)	5	Zella, L.	25-May	2:30PM	Constellation F (Second floor)	17
Rouxel, T.	23-May	2:30PM	Frederick (Second floor)	6	Zhang, F.	25-May	9:20AM	Columbia (Second floor)	15
Rouxel, T.	25-May	2:50PM	Frederick (Second floor)	17	Zhang, Y.	24-May	2:20PM	Frederick (Second floor)	13
Ryan, J.V.	23-May	11:30AM	Constellation C/D (Second floor)	4	Zhang, Y.	24-May	2:40PM	Frederick (Second floor)	13
		<b>S</b>			Zhang, Y.	26-May	10:40AM	Frederick (Second floor)	19
Sargin, I.	24-May	1:20PM	Frederick (Second floor)	13	Zhou, S.	23-May	1:20PM	Columbia (Second floor)	7
Schaut, R.	26-May	9:20AM	Constellation F (Second floor)	18					
Schuller, S.	24-May	10:50AM	Constellation F (Second floor)	12					
Sen, S.	24-May	10:10AM	Columbia (Second floor)	10					
Shasmal, N.	23-May	10:10AM	Constellation E (Second floor)	5					
Shi, W.	23-May	3:20PM	Columbia (Second floor)	7					
Shi, Y.	24-May	11:40AM	Constellation E (Second floor)	10					
Shi, Y.	24-May	2:30PM	Columbia (Second floor)	13					
Sidebottom, D.	24-May	3:00PM	Constellation E (Second floor)	12					
Singla, S.	23-May	2:20PM	Columbia (Second floor)	7					
Smedskjaer, M.M.	23-May	9:20AM	Frederick (Second floor)	4					
Smedskjaer, M.M.	24-May	11:20AM	Constellation E (Second floor)	10					
Smith-Gray, N.J.	24-May	10:10AM	Frederick (Second floor)	11					
Smith, N.J.	23-May	9:20AM	Constellation C/D (Second floor)	4					
Smith, N.J.	26-May	9:50AM	Constellation F (Second floor)	18					
Sokmen, I.	23-May	1:20PM	Constellation F (Second floor)	8					



Poster Presenters

<u>Name</u>	<u>Date</u>	<u>Time</u>	<u>Room</u>	<u>Page Number</u>	<u>Name</u>	<u>Date</u>	<u>Time</u>	<u>Room</u>	<u>Page Number</u>
<b>A</b>					<b>M</b>				
Astle, S.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	Meehan, B.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
<b>B</b>					<b>O</b>				
Bussey, J.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Okkema, M.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
<b>C</b>					<b>P</b>				
Cahoon, M.A.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Philipp, P.J.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
Caurant, D.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	<b>R</b>				
Cowen, A.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	Read, A.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
<b>D</b>					<b>S</b>				
Diaw, A.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Sahoo, S.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
Dong, G.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Shirshnev, P.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
<b>E</b>					<b>T</b>				
Erickson, J.J.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Sørensen, S.S.	23-May	6:30PM	Atrium/Harborview (Second floor)	8
<b>F</b>					<b>U</b>				
Fettkether, W.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Stone, M.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
Franklin, J.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Tsekrekas, E.M.	23-May	6:30PM	Atrium/Harborview (Second floor)	8
<b>G</b>					<b>V</b>				
Gervasio, V.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Uppala, H.	23-May	6:30PM	Atrium/Harborview (Second floor)	8
Greiner, L.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	<b>W</b>				
Guthrie, W.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Vacchi, M.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
<b>H</b>					<b>Y</b>				
Hauke, B.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	Vasquez, A.	23-May	6:30PM	Atrium/Harborview (Second floor)	8
Hyun, S.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	<b>Y</b>				
<b>K</b>					<b>Y</b>				
Keith, T.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	White, S.S.	23-May	6:30PM	Atrium/Harborview (Second floor)	9
<b>L</b>					<b>Y</b>				
Leland, S.J.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	Yin, T.	23-May	6:30PM	Atrium/Harborview (Second floor)	8
Lere-Adams, A.J.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	<b>Y</b>				
Lewis, T.C.	23-May	6:30PM	Atrium/Harborview (Second floor)	8	<b>Y</b>				
Lumpkin, D.C.	23-May	6:30PM	Atrium/Harborview (Second floor)	9	<b>Y</b>				

## Monday, May 23, 2022

### Award Lectures

#### Stookey Lecture of Discovery

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

**8:00 AM**

#### Introduction

**8:10 AM**

#### (GOMD-AW-001-2022) Nanostructured Glasses (Nano-glasses): The Door to a New Glass-based Technology Age: A Glass Age

H. Gleiter\*<sup>1</sup>

1. Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Germany

**8:50 AM**

#### Award Presentation

### S1: Fundamentals of the Glassy State

#### Mechanical Properties of Glasses: Indentation Responses

Room: Frederick (Second floor)

Session Chair: Satoshi Yoshida, AGC Inc.

**9:20 AM**

#### (GOMD-S1-001-2022) Fracture and Bond Switching in Simulated Glassy Alumina and Silica

M. M. Smedskjaer\*<sup>1</sup>; T. Du<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

**9:40 AM**

#### (GOMD-S1-002-2022) Impact of pressure on the structure and properties of metaluminous sodium aluminoborosilicate glasses

N. Stone-Weiss\*<sup>2</sup>; B. Siboczy<sup>1</sup>; R. Sun<sup>3</sup>; N. J. Smith<sup>2</sup>; R. Youngman<sup>2</sup>; M. Bockowski<sup>4</sup>; L. Huang<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Materials Science and Engineering, USA
2. Corning Incorporated, Science and Technology Division, USA
3. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
4. Institute of Physics Polish Academy of Sciences, Institute of High Pressure Physics, Poland

**10:00 AM**

#### (GOMD-S1-003-2022) Correlation of hardness of aluminosilicates and glass network connectivity and atomic packing density

H. Lee\*<sup>1</sup>; W. M. Carty<sup>1</sup>

1. Alfred University, New York State college of ceramics at Alfred University, USA

**10:20 AM**

#### (GOMD-S1-004-2022) Impact of modifier field strength on hardness, crack resistance, and charge distribution in single modifier aluminoborosilicate glasses

A. L. Fry\*<sup>4</sup>; I. Slagle<sup>2</sup>; H. Hawbaker<sup>2</sup>; C. George<sup>3</sup>; S. Feller<sup>2</sup>; S. H. Kim<sup>1</sup>; J. C. Mauro<sup>4</sup>

1. Pennsylvania State University, Chemical Engineering, USA
2. Coe College, Physics, USA
3. Pennsylvania State University, Chemistry, USA
4. Pennsylvania State University, Materials Science and Engineering, USA

**10:40 AM**

#### (GOMD-S1-005-2022) Hard and crack-resistant glass

A. Yadav\*<sup>1</sup>; A. Goel<sup>1</sup>

1. Rutgers, The State University of New Jersey, Materials Science & Engineering, USA

**11:00 AM**

#### (GOMD-S1-006-2022) Lateral-pushing induced surface lift-up during nanoindentation of silicate glass

L. Ding\*<sup>1</sup>; Q. Zheng<sup>2</sup>; J. C. Mauro<sup>3</sup>

1. Donghua University, College of Materials Science and Engineering, China
2. Qilu University of Technology, School of Materials Science and Engineering, China
3. The Pennsylvania State University, Department of Materials Science and Engineering, USA

**11:20 AM**

#### (GOMD-S1-007-2022) 3D Raman Mapping of Glass Indentation Stress Fields

A. J. Bellafatto\*<sup>1</sup>; I. Reimanis<sup>1</sup>

1. Colorado School of Mines, Materials Science, USA

**11:40 AM**

#### (GOMD-S1-008-2022) Crack nucleation and propagation mechanisms in amorphous silica

Z. Hossain\*<sup>1</sup>

1. University of Delaware, Mechanical Engineering, USA

### S2: Glass and Interactions with Its Environment: Fundamentals and Applications

#### Dissolution and Interfacial Reactions I: Dissolution behavior as a Function of Glass Composition

Room: Constellation C/D (Second floor)

Session Chairs: Alfonso Pedone, University of Modena and Reggio Emilia; Stéphane Gin, CEA

**9:20 AM**

#### (GOMD-S2-001-2022) The Composition Dependence of Glass Dissolution Rate (Invited)

N. J. Smith\*<sup>2</sup>; R. Schaut<sup>1</sup>; E. Bakowska<sup>1</sup>; J. P. Icenhower<sup>1</sup>; A. Tandia<sup>1</sup>; S. Goyal<sup>1</sup>; R. Youngman<sup>1</sup>

1. Corning Incorporated, USA

**9:50 AM**

#### (GOMD-S2-002-2022) Deciphering the non-linear impact of Al on chemical durability of silicate glass

K. Damodaran\*<sup>1</sup>; J. Delaye<sup>1</sup>; A. Kalinichev<sup>1</sup>; S. Gin<sup>1</sup>

1. CEA, France

**10:10 AM**

#### (GOMD-S2-003-2022) Glass Formation and Chemical Durability in Copper Borates

C. Calahoo\*<sup>1</sup>; P. N. DeMaere<sup>1</sup>; S. Adab<sup>2</sup>; Y. Boluk<sup>1</sup>; W. Wall<sup>2</sup>

1. University of Alberta, Civil Engineering, Canada
2. Genics Inc., Canada

**10:30 AM**

#### (GOMD-S2-004-2022) Structure of Calcium Aluminosilicate Glasses and its Role in Governing Dissolution Kinetics

J. P. Icenhower\*<sup>1</sup>; N. J. Smith<sup>2</sup>; R. Youngman<sup>2</sup>; D. K. Shuh<sup>3</sup>; H. McMahon<sup>1</sup>; M. Riesbeck<sup>1</sup>

1. Corning Incorporated, Chemical Analysis, USA
2. Corning Incorporated, USA
3. Lawrence Berkeley National Laboratory, USA

**10:50 AM**

#### (GOMD-S2-005-2022) Dissolution behavior and kinetics of alkali/alkaline-earth aluminoborosilicate glasses in acidic media: Impact of high ionic field strength non-framework cations

Q. Qin\*<sup>1</sup>; N. Stone-Weiss<sup>1</sup>; T. Zhao<sup>2</sup>; P. Mukherjee<sup>2</sup>; J. Ren<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Michigan Technological University, Materials Science and Engineering, USA
3. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Key Laboratory of Materials for High-Power Laser, China

**11:10 AM**

#### (GOMD-S2-006-2022) Dissolution Reaction Products from Na<sub>2</sub>O-CaO-B<sub>2</sub>O<sub>3</sub>-P<sub>2</sub>O<sub>5</sub> Glasses in Simulated Body Fluids

R. L. Blatt\*<sup>1</sup>; R. Brow<sup>1</sup>

1. Missouri University of Science & Technology, Materials Science and Engineering, USA

**11:30 AM**

#### (GOMD-S2-007-2022) Stirred Reactor Coupon Analysis – A Round Robin Study

J. V. Ryan\*<sup>1</sup>; B. Parruzot<sup>2</sup>; J. Reiser<sup>2</sup>; S. Cooley<sup>2</sup>; D. Swanberg<sup>3</sup>; G. L. Smith<sup>2</sup>

1. Pacific Northwest National Lab, Advanced Processing and Applications, USA
2. Pacific Northwest National Lab, Energy and Environment, USA
3. Washington River Protection Systems, USA

**Glasses and Glass-ceramics for Healthcare**

Room: Columbia (Second floor)

Session Chair: Hrishikesh Kamat, Glidewell Dental

**9:20 AM****(GOMD-S2-008-2022) Multifunctional bioactive glasses doped with therapeutic ions/nanoparticles (Invited)**M. Miola<sup>1</sup>; E. Verné<sup>\*1</sup>

1. Politecnico di Torino, DISAT, Italy

**9:50 AM****(GOMD-S2-009-2022) Glass-Ceramic Scintillators for Indirect Digital Radiography**E. Moore<sup>\*1</sup>; R. L. Leonard<sup>1</sup>; J. A. Johnson<sup>1</sup>; A. M. Thomas<sup>1</sup>; A. R. Lubinsky<sup>2</sup>; A. Howansky<sup>2</sup>

1. University of Tennessee Space Institute, MABE, USA
2. Stony Brook University, USA

**10:10 AM****(GOMD-S2-010-2022) Human Adipose Stem Cells Viability on Ag-doped Bioactive Glass Obtained by Ion Exchange**M. S. Lallukka<sup>\*1</sup>; A. Houaoui<sup>2</sup>; M. Miola<sup>1</sup>; J. Massera<sup>2</sup>; E. Verné<sup>1</sup>

1. Politecnico di Torino, Department of Applied Science and Technology, Italy
2. Tampere University, Faculty of Medicine and Health Technology, Finland

**10:30 AM****(GOMD-S2-011-2022) Bioactive sol-gel borate glasses for regenerative engineering (Invited)**W. C. Lepry<sup>1</sup>; S. Naseri<sup>1</sup>; E. Rezabeigi<sup>1</sup>; S. N. Nazhat<sup>\*1</sup>

1. McGill University, Mining and Materials Engineering, Canada

**11:00 AM****(GOMD-S2-012-2022) Tribo-corrosion Studies of 45S5 Bioglass in Aqueous Media**S. R. Keshri<sup>\*1</sup>; S. Sahoo<sup>1</sup>; K. S<sup>1</sup>; N. Krishnan<sup>2</sup>; N. N. Gosvami<sup>1</sup>

1. Indian Institute of Technology Delhi, Materials Science & Engineering, India
2. Indian Institute of Technology Delhi, Civil Engineering, India

**11:20 AM****(GOMD-S2-013-2022) Sol-gel synthesis of spherical bioactive glass particles containing boron and copper**E. Piatti<sup>\*1</sup>; M. Miola<sup>1</sup>; E. Verné<sup>1</sup>

1. Politecnico di Torino, Department of Applied Science and Technology, Italy

**11:40 AM****(GOMD-S2-014-2022) Synthesizing Nanocerium with Varied Ratios of Ce<sup>3+</sup>/Ce<sup>4+</sup> Using Soluble Borate Glass**K. S. Ranasinghe<sup>\*1</sup>; R. Singh<sup>2</sup>; A. Vasquez<sup>2</sup>

1. Kennesaw State University, Physics, USA
2. Kennesaw State University, Chemistry and Biochemistry, USA

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Optical and Photonic Glasses and Glass-ceramics I**

Room: Constellation E (Second floor)

Session Chair: Lee Casalena

**9:20 AM****(GOMD-S3-001-2022) Glass-ceramics or composites for infrared luminescence properties (Invited)**V. Jubera<sup>\*1</sup>

1. Université de Bordeaux, ICMCB, France

**9:50 AM****(GOMD-S3-002-2022) Luminescent properties of nanostructured glass-ceramic thin films and their potential for UV-pumped white light LED applications**R. L. Leonard<sup>\*1</sup>; C. W. Bond<sup>1</sup>; Y. Jin<sup>4</sup>; P. Gómez-Rodríguez<sup>2</sup>; E. Nieto<sup>3</sup>; J. Gonzalo<sup>3</sup>; R. Serna<sup>3</sup>; A. Petford-Long<sup>2</sup>; J. A. Johnson<sup>1</sup>

1. University of Tennessee Space Institute, Mechanical, Aerospace, and Biomedical Engineering, USA
2. Argonne National Laboratory, Materials Science Division, USA
3. Instituto de Optica CSIC, Laser Processing Group, Spain
4. Northwestern University, Materials Science and Engineering, USA

**10:10 AM****(GOMD-S3-003-2022) Photoluminescence Enhancement in Eu/CdS co-doped chloroborosilicate glass-ceramics by heat treatment**N. Shasmal<sup>\*1</sup>; W. G. Faria<sup>2</sup>; A. S. de Camargo<sup>2</sup>; A. Rodrigues<sup>1</sup>

1. Federal University of Sao Carlos, LaMaV, Brazil
2. University of São Paulo, São Carlos Institute of Physics, LEMAF – Laboratório de Espectroscopia de Materiais Funcionais, Brazil

**10:30 AM****(GOMD-S3-004-2022) Novel oxide glasses via non-traditional processing**A. Floyd<sup>\*1</sup>; V. Nguyen<sup>1</sup>; R. Bekele<sup>2</sup>; J. Myers<sup>3</sup>; D. Gibson<sup>3</sup>; S. Bayya<sup>3</sup>; W. Kim<sup>1</sup>; J. Frantz<sup>4</sup>; D. Rhonehouse<sup>2</sup>; J. Sanghera<sup>2</sup>

1. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5621, USA
2. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5620, USA
3. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5622, USA
4. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5624, USA
5. Jacobs, On-site contractor for NRL Code 5622, USA
6. University Research Foundation, On-site contractor for NRL Code 5624, USA

**10:50 AM****(GOMD-S3-005-2022) Structure analysis of CaO-WO<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> glass and thermal evolution to Glass-Ceramics bearing Calcium Tungstate crystals with enhancement photoluminescence by Eu<sup>3+</sup> doping**T. Otsuka<sup>\*1</sup>; M. Brehl<sup>2</sup>; M. Cicconi<sup>2</sup>; D. de Ligny<sup>2</sup>; T. Hayakawa<sup>1</sup>

1. Nagoya Institute of Technology, Life Science and Applied Chemistry, Japan
2. University of Erlangen-Nuremberg, Department of Materials Science and Engineering, Germany

**11:10 AM****(GOMD-S3-006-2022) The role of powder handling on resulting impurities in ZnSe-doped As-S-Se composite materials**A. Kostogiannes<sup>\*1</sup>; R. Sharma<sup>1</sup>; M. Chazot<sup>1</sup>; M. Kang<sup>1</sup>; C. Blanco<sup>1</sup>; J. Cook<sup>1</sup>; V. Rodriguez<sup>2</sup>; F. Adamietz<sup>2</sup>; D. Verrault<sup>2</sup>; K. Schepler<sup>1</sup>; M. Richardson<sup>1</sup>; K. A. Richardson<sup>1</sup>

1. University of Central Florida, CREOL, USA
2. University Bordeaux, France

**S4: Glass Technology and Cross-Cutting Topics****Green Manufacturing**

Room: Constellation F (Second floor)

Session Chairs: Laura Adkins, Corning Research and Development Corporation; Irene Peterson, Corning Incorporated

**9:20 AM****(GOMD-S4-001-2022) A Review of the Challenges for Melting Reduced Container Glass Colors in Cold Top All-Electric Furnaces (Invited)**C. P. Ross<sup>\*1</sup>

1. GICI, USA

**9:50 AM****(GOMD-S4-002-2022) Hydrogen as a fuel for glass production (Invited)**O. Verheijen<sup>\*1</sup>

1. CelSian Glass & Solar, Netherlands



**10:20 AM****(GOMD-S4-003-2022) Furnace of the future, strategies for carbon reduction (Invited)**E. H. Muijsenberg\*<sup>1</sup>

1. Glass Service, Czechia

**10:50 AM****(GOMD-S4-004-2022) Immersed Radiant Heater - A unique heat source for glass melting (Invited)**T. Maehara\*<sup>1</sup>; A. Niwa<sup>1</sup>; S. Hyodo<sup>1</sup>; T. Enomoto<sup>1</sup>; T. Yamazaki<sup>1</sup>; Y. Doi<sup>1</sup>; L. Keen<sup>2</sup>; R. Pauli<sup>2</sup>

1. AGC Inc., Innovative Technology Laboratories, Japan
2. Apollo Furnaces Ltd., United Kingdom

**11:20 AM****(GOMD-S4-005-2022) Oolitic Aragonite: A Renewable and Sustainable Solution for High Clarity Glass Manufacturing**A. J. Myers\*<sup>1</sup>

1. Calcean Minerals & Materials LLC, USA

**S1: Fundamentals of the Glassy State****Mechanical Properties of Glasses: Fracture and Crack Propagation**

Room: Frederick (Second floor)

Session Chair: Morten Smedskjaer, Aalborg University

**1:20 PM****(GOMD-S1-009-2022) Slow Crack Growth in Sodium-Modified Silicate Glasses (Invited)**J. M. Rimsza\*<sup>1</sup>; K. T. Strong<sup>1</sup>; C. Nakakura<sup>1</sup>; J. Duree<sup>1</sup>; K. Stephens<sup>1</sup>; S. Grutzki<sup>1</sup>

1. Sandia National Laboratories, USA

**1:50 PM****(GOMD-S1-010-2022) A Comparison of Subcritical Crack Growth Behavior and the Dynamic Fatigue Parameter of Alkali Silicate Glasses**N. Weyrauch\*<sup>1</sup>; R. Brown<sup>1</sup>; K. T. Strong<sup>2</sup>; G. Miller<sup>1</sup>; T. Diebold<sup>2</sup>

1. Missouri University of Science & Technology, Material Science and Engineering, USA
2. Sandia National Laboratories, Material Mechanics and Tribology, USA

**2:10 PM****(GOMD-S1-011-2022) Origin of Region II Slow Crack Growth of Oxide Glasses**Z. Huang\*<sup>1</sup>; M. Tomozawa<sup>1</sup>

1. Rensselaer Polytechnic Institute, Materials Science & Engineering, USA

**2:30 PM****(GOMD-S1-012-2022) Elaboration and fracture properties of glass matrix/glass particles composites**T. Rouxel\*<sup>1</sup>; T. Lacondemine<sup>1</sup>; F. C elari e<sup>1</sup>; P. Houizot<sup>1</sup>

1. Universit e de Rennes 1, Glass Mechanics, France

**2:50 PM****(GOMD-S1-013-2022) Effect of Local Residual Stress on Fractal Dimension of Silicate Glasses**J. Mecholsky\*<sup>1</sup>; J. Chan<sup>1</sup>

1. University of Florida, Materials Science & Engineering, USA

**3:10 PM****Break****3:30 PM****(GOMD-S1-014-2022) Residual Stress resulting from ion exchange in silicate glasses (Invited)**G. Macrelli\*<sup>1</sup>

1. Isoclima SpA, R&D, Italy

**4:00 PM****(GOMD-S1-015-2022) Fracture Mechanism Analysis of Ultra-Thin Glass for Flexible Display Cover Window**S. Kim\*<sup>1</sup>; W. Chung<sup>2</sup>; G. Shim<sup>1</sup>; S. Jung<sup>1</sup>; H. Sohn<sup>1</sup>; S. Kim<sup>1</sup>

1. Samsung Display Co. Ltd., Republic of Korea
2. Kongju National University, Institute for Rare Metals & Division of Advanced Materials Engineering, Republic of Korea

**S2: Glass and Interactions with Its Environment: Fundamentals and Applications****Dissolution and Interfacial Reactions II: Long-term Corrosion and Nuclear Waste Glasses**

Room: Constellation C/D (Second floor)

Session Chairs: Jon Icenhower, Corning Incorporated; Jincheng Du, University of North Texas

**1:20 PM****(GOMD-S2-015-2022) Long Term Corrosion Interactions between Stainless Steel and International Simple Glass (Invited)**C. Mohanty<sup>1</sup>; X. Guo\*<sup>1</sup>; H. Kaya<sup>2</sup>; S. Gin<sup>3</sup>; K. Yang<sup>4</sup>; Z. Zhang<sup>5</sup>; S. H. Kim<sup>5</sup>; J. Lian<sup>2</sup>; J. Wang<sup>5</sup>; G. Frankel<sup>1</sup>

1. Ohio State University, Materials Science and Engineering, USA
2. Pennsylvania State University, Chemical Engineering and Materials Research Institute, USA
3. CEA, DE2D, France
4. Rensselaer Polytechnic Institute, Mechanical Aerospace and Nuclear Engineering, USA
5. Louisiana State University, Geology and Geophysics, USA

**1:50 PM****(GOMD-S2-016-2022) Applying laboratory methods for durability assessment of vitrified material to archaeological samples**J. Neeway\*<sup>1</sup>; J. Marcial<sup>1</sup>; L. Nava-Farias<sup>1</sup>; C. Pearce<sup>1</sup>; D. Peeler<sup>1</sup>; C. L. Thorpe<sup>2</sup>; C. L. Corkhill<sup>2</sup>; R. J. Hand<sup>2</sup>; D. Kosson<sup>2</sup>; R. Delapp<sup>2</sup>; A. A. Kruger<sup>4</sup>

1. Pacific Northwest National Lab, USA
2. Sheffield University, United Kingdom
3. Vanderbilt University, USA
4. US Department of Energy, USA

**2:10 PM****(GOMD-S2-017-2022) Long-term dissolution of simulated UK Ca/Zn HLW glass in conditions relevant to disposal**M. T. Harrison\*<sup>1</sup>; T. Taylor<sup>1</sup>

1. National Nuclear Laboratory, WM&D, United Kingdom

**2:30 PM****(GOMD-S2-018-2022) Insights into the mechanisms controlling the residual corrosion rate of borosilicate glasses**S. Gin\*<sup>1</sup>; X. Guo<sup>2</sup>; J. Delaye<sup>1</sup>; F. Angeli<sup>1</sup>; K. Damodaran<sup>1</sup>; S. H. Kim<sup>3</sup>

1. CEA, DE2D, France
2. Ohio State University, USA
3. Pennsylvania State University, USA

**2:50 PM****(GOMD-S2-019-2022) Dissolution rate of a simulated nuclear waste glass ISG as a function of solution concentration of Si and pH**Y. Inagaki\*<sup>1</sup>

1. Kyushu University, Department of Applied Quantum Physics & Nuclear Engineering, Japan

**3:10 PM****Break****3:30 PM****(GOMD-S2-020-2022) Application of the Immobilized Low-Activity Waste Glass Corrosion Model to the Static Dissolution of Enhanced Waste Glasses (Invited)**S. N. Kerisit\*<sup>1</sup>; J. Neeway<sup>2</sup>; C. Lonergan<sup>2</sup>; B. Parruzot<sup>2</sup>; J. V. Crum<sup>2</sup>; J. V. Ryan<sup>2</sup>; M. Asmussen<sup>2</sup>; G. L. Smith<sup>2</sup>

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA
2. Pacific Northwest National Lab, Energy and Environment Directorate, USA

**4:00 PM****(GOMD-S2-021-2022) Improvements to the Immobilized Low-Activity Waste Glass Corrosion Model for the Hanford Site Integrated Disposal Facility**

J. Neeway\*<sup>1</sup>; C. Lonergan<sup>1</sup>; S. N. Kerisit<sup>1</sup>; B. Parruzot<sup>1</sup>; J. V. Crum<sup>1</sup>; J. V. Ryan<sup>1</sup>; M. Assmusen<sup>1</sup>; G. L. Smith<sup>1</sup>; D. Swanberg<sup>2</sup>; R. Skeen<sup>2</sup>

1. Pacific Northwest National Lab, USA
2. Washington River Protection Solutions, USA

**4:20 PM****(GOMD-S2-022-2022) R&D program of operational model of long-term performance for vitrified High-level Radioactive Waste**

R. Matsubara\*<sup>1</sup>

1. Nuclear Waste Management Organization of Japan, Science and Technology Department, Japan

**4:40 PM****(GOMD-S2-023-2022) The impact of AI on the chemical durability of pristine and irradiated borosilicate glasses**

A. Jan<sup>1</sup>; J. Delaye\*<sup>1</sup>; K. Damodaran<sup>1</sup>; S. N. Kerisit<sup>2</sup>; M. Tribet<sup>1</sup>; S. Gin<sup>1</sup>

1. CEA Marcoule, DE2D, France
2. Pacific Northwest National Laboratory, Physical and Computational Sciences Directorate, USA

**5:00 PM****(GOMD-S2-024-2022) Impact of irradiation on the properties of calcium silicate hydrate (CSH) gel layer formed after aqueous corrosion of borosilicate glasses**

A. Jan\*<sup>1</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, India

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Glass-based Photonics I: Bulk and Fiber Devices**

Room: Columbia (Second floor)

Session Chairs: Juejun Hu, Massachusetts Institute of Technology; Hongtao Lin, Massachusetts Institute of Technology

**1:20 PM****(GOMD-S3-007-2022) Multicomponent Photonic Glass Fibers and Devices (Invited)**

S. Zhou\*<sup>1</sup>

1. South China University of Technology, School of Materials Science and Engineering, China

**1:50 PM****(GOMD-S3-008-2022) Luminescent glass-based materials development for photonics and biophotonics applications (Invited)**

L. Petit\*<sup>1</sup>

1. Tampere University, Finland

**2:20 PM****(GOMD-S3-009-2022) Bismuth Borosilicate glass containing Eu<sub>2</sub>O<sub>3</sub> stabilized gold nanoparticles with high third-order nonlinearity**

S. Singla\*<sup>1</sup>; V. G. Achanta<sup>2</sup>; O. P. Pandey<sup>3</sup>; G. Sharma<sup>4</sup>

1. Chandigarh University, Physics Department, India
2. NPL, India
3. Thapar Institution of Engineering & Technology, India
4. KMV College, India

**2:40 PM****(GOMD-S3-010-2022) Progress towards the development of advanced freeform glass optics**

T. I. Suratwala\*<sup>1</sup>; J. A. Menapace<sup>1</sup>; G. Tham<sup>1</sup>; W. A. Steele<sup>1</sup>; N. Ray<sup>1</sup>; L. L. Wong<sup>1</sup>; B. Bauman<sup>1</sup>

1. Lawrence Livermore National Laboratory, USA

**3:00 PM****Break****Glass-based Photonics II: Planar Devices**

Room: Columbia (Second floor)

Session Chairs: Hongtao Lin, Massachusetts Institute of Technology; Juejun Hu, Massachusetts Institute of Technology

**3:20 PM****(GOMD-S3-011-2022) Self-assembled chalcogenide photonic integrated circuits on silicon (Invited)**

W. Shi\*<sup>1</sup>; P. Jean<sup>1</sup>; A. Douaud<sup>2</sup>; S. Laroche<sup>2</sup>; Y. Messaddeq<sup>2</sup>

1. Université Laval, Department of Electrical and Computer Engineering, Canada
2. Université Laval, Center for Optics, Photonics, and Lasers, Canada

**3:50 PM****(GOMD-S3-012-2022) Phase change material enabled parafocal zoom metalens**

J. Hu\*<sup>1</sup>

1. Massachusetts Institute of Technology, USA

**4:10 PM****(GOMD-S3-013-2022) Phase change material based metasurfaces on a foundry-processed silicon-on-insulator platform**

C. Popescu\*<sup>1</sup>; Y. Zhang<sup>1</sup>; C. Rios<sup>2</sup>; Q. Du<sup>1</sup>; L. Martin-Monier<sup>1</sup>; L. Ranno<sup>1</sup>; M. Shalaginov<sup>1</sup>; P. Miller<sup>3</sup>; C. Roberts<sup>3</sup>; M. Kang<sup>3</sup>; K. A. Richardson<sup>3</sup>; T. Gu<sup>1</sup>; S. Vitale<sup>2</sup>; J. Hu<sup>1</sup>

1. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA
2. University of Maryland, Department of Materials Science and Engineering, USA
3. Massachusetts Institute of Technology, Lincoln Laboratory, USA
4. University of Central Florida, The College of Optics and Photonics, Department of Materials Science and Engineering, USA

**4:30 PM****(GOMD-S3-014-2022) Flexible glass integrated photonic devices with superior optical and mechanical performance**

Y. Luo\*<sup>1</sup>; C. Sun<sup>1</sup>; H. Ma<sup>2</sup>; M. Wei<sup>2</sup>; J. Li<sup>2</sup>; J. Jian<sup>1</sup>; C. Zhong<sup>2</sup>; Z. Chen<sup>1</sup>; R. Tang<sup>1</sup>; K. A. Richardson<sup>3</sup>; H. Lin<sup>2</sup>; L. Li<sup>1</sup>

1. Westlake University, School of Engineering, China
2. Zhejiang University, College of Information Science and Electronic Engineering, China
3. University of Central Florida, Department of Materials Science & Engineering, USA

**Optical and Photonic Glasses and Glass-ceramics II**

Room: Constellation E (Second floor)

Session Chair: Russell Leonard, University of Tennessee Space Institute

**1:20 PM****(GOMD-S3-015-2022) Waveguides based on germanate and tellurite glasses fabricated with Si technology and fs laser writing techniques for IR applications: A review (Invited)**

L. R. Kassab\*<sup>1</sup>

1. Faculty of Technology of Sao Paulo, Departamento de Ensino Geral, Brazil

**1:50 PM****(GOMD-S3-016-2022) Effect of UV exposure and low temperature treatment on optical properties of Photo-Thermo-Refractive glass**

R. Alvarez\*<sup>1</sup>; D. C. Lumpkin<sup>1</sup>; P. Shirshnev<sup>1</sup>; A. Rysanskiy<sup>2</sup>; L. Glebov<sup>1</sup>

1. University of Central Florida, CREOL, USA
2. Optigrate Corp., USA

**2:10 PM****(GOMD-S3-017-2022) Ultraviolet Opacification of Ce-Mn Codoped Silicate Glass**

C. Bellows\*<sup>1</sup>; A. G. Clare<sup>1</sup>

1. Alfred University, USA

**2:30 PM****(GOMD-S3-018-2022) 2D and 3D Structural Evolution and Chemical Characterization of Nanoparticles in Fiber Optics**

H. Francois-Saint-Cyr<sup>1</sup>; R. Passey<sup>1</sup>; C. Guillemier<sup>2</sup>; I. Martin<sup>3</sup>; L. Casalena\*<sup>1</sup>; J. Ballato<sup>4</sup>; P. Le Coustumer<sup>2</sup>; W. Blanc<sup>6</sup>

1. Thermo Fisher Scientific, Materials and Structural Analysis Division, USA
1. Harvard Medical School/Brigham and Women's Hospital, USA
3. CAMECA, USA
4. Clemson University, USA
5. University of Bordeaux, France
6. Institut de Physique de Nice, France

**2:50 PM****(GOMD-S3-019-2022) Atomistic Simulation Study of Li-Aluminosilicate Glass Scintillators**

E. Ghardji\*

1. Bangor University, Nuclear Future Institute, United Kingdom

**3:10 PM****(GOMD-S3-020-2022) Glasses for multiband visible/IR optics**D. Gibson<sup>3</sup>; W. Kim<sup>\*1</sup>; V. Nguyen<sup>1</sup>; K. Major<sup>2</sup>; A. Floyd<sup>4</sup>; S. Bayya<sup>3</sup>; J. Sanghera<sup>1</sup>

1. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5621, USA
2. US Naval Research Laboratory, Optical Sciences Division - Code 5623, USA
3. US Naval Research Laboratory, Optical Sciences Division - Code 5622, USA
4. Jacobs, On-site contractor for NRL Code 5622, USA

**S4: Glass Technology and Cross-Cutting Topics****Forming and Coatings**

Room: Constellation F (Second floor)

Session Chairs: Jennifer Rygel, Corning Incorporated; Irene Peterson, Corning Incorporated

**1:20 PM****(GOMD-S4-006-2022) Scalable Deposition of Durable Antimicrobial Thin Film Coatings on Complex Shaped Glass Substrates (Invited)**I. Sokmen<sup>\*1</sup>; B. Okan<sup>1</sup>; H. Erdem<sup>1</sup>; R. Budakoğlu<sup>1</sup>; G. Aydın<sup>1</sup>; Z. Aydın<sup>1</sup>; A. Özen<sup>1</sup>

1. Türkiye Sise ve Cam Fabrikalari A.S., Science Technology and Design Center, Turkey

**1:50 PM****(GOMD-S4-007-2022) Latest Development in Hot Forming of 3D Shaped Thin Glass Components for Mass Production**P. Vogel<sup>\*1</sup>; A. Vu<sup>1</sup>; C. Strobl<sup>1</sup>; T. Grunwald<sup>1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer Institute for Production Technology IPT, Fine Machining and Optics, Germany
2. Laboratory for Machine Tools WZL RWTH Aachen University, Germany

**2:10 PM****(GOMD-S4-009-2022) Enabling energy- and cost-efficient production of glass optics by non-isothermal wafer-level glass molding**C. Strobl<sup>\*1</sup>; P. Vogel<sup>1</sup>; A. Vu<sup>1</sup>; T. Grunwald<sup>1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer Institute for Production Technology, Fine Machining and Optics, Germany
2. RWTH Aachen University, Laboratory for Machine Tools WZL, Germany

**2:30 PM****(GOMD-S4-010-2022) Monte-Carlo simulation based wear prediction for Precision Glass Molding of fused silica**T. Grunwald<sup>\*1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer IPT, Fine Machining and Optics, Germany
2. WZL Tool Machine Laboratory of RWTH Aachen University, Chair for Manufacturing Technology, Germany

**2:50 PM****Break****Glass Challenges**

Room: Constellation F (Second floor)

Session Chairs: Jennifer Rygel, Corning Incorporated; Irene Peterson, Corning Incorporated

**3:40 PM****(GOMD-S4-012-2022) Conference on Glass Problems – Sharing Glass Manufacturing Innovations and Educating the Next Generation of Glass Engineers**S. K. Sundaram<sup>\*1</sup>; R. Lipetz<sup>2</sup>

1. Alfred University, Inamori School of Engineering, USA
2. Glass Manufacturing Industry Council, USA

**4:00 PM****(GOMD-S4-013-2022) GlassArtEngine – Teaching Across Glass Arts, Science, and Engineering**C. Bellows<sup>1</sup>; E. M. Tsekrekas<sup>1</sup>; D. Möncke<sup>\*1</sup>; A. G. Clare<sup>1</sup>; S. K. Sundaram<sup>1</sup>; A. Powers<sup>2</sup>

1. Alfred University, Inamori School of Engineering, USA
2. Alfred University, School of Arts and Design, USA

**Poster Session**

Room: Atrium/Harborview (Second floor)

**6:30 PM****(GOMD-S1-SP001-2022) Impact of a Temperature-Dependent Stretching Exponent on Glass Relaxation**B. Hauke<sup>\*1</sup>; M. Mancini<sup>1</sup>; J. C. Mauro<sup>1</sup>

1. Pennsylvania State University, MatSE, USA

**(GOMD-S1-SP002-2022) Dynamic Light Scattering in Potassium Borate Glass Melts**H. Uppala<sup>\*1</sup>; D. Sidebottom<sup>1</sup>

1. Creighton University, Physics, USA

**(GOMD-S1-SP003-2022) NMR Investigations of the Structural Role of Phosphorous in Aluminosilicate Glasses for Ion Exchange**A. Cowen<sup>\*1</sup>; M. Bovee<sup>2</sup>; D. Srivastava<sup>2</sup>; J. Wu<sup>1</sup>; P. J. Grandinetti<sup>2</sup>

1. Ohio State University, Materials Science and Engineering, USA
2. Ohio State University, Department of Chemistry, USA
3. Corning Incorporated, Glass Research, USA

**(GOMD-S1-SP004-2022) Alkali Tungsten-Borate: Investigation of Structure and Properties**E. M. Tsekrekas<sup>\*1</sup>; A. G. Clare<sup>1</sup>

1. Alfred University, Glass Science, USA

**(GOMD-S1-SP005-2022) Oxygen Triclusters and Five-Coordinated Alumina Species in Calcium-aluminosilicate Glasses**S. Astle<sup>\*1</sup>; R. Welch<sup>1</sup>; J. C. Mauro<sup>1</sup>

1. Pennsylvania State University, Materials Science and Engineering, USA

**(GOMD-S1-SP006-2022) Untypical blue colors in glasses with varying optical basicity**L. Greiner<sup>\*1</sup>; J. Kasprzyk<sup>1</sup>; D. Möncke<sup>1</sup>

1. Alfred University, Glass, USA

**(GOMD-S1-SP008-2022) Structural Evidence of Mixed Alkali Effect for Aluminoborosilicate Glasses**S. Hyun<sup>\*1</sup>; J. Cho<sup>1</sup>

1. Pohang University of Science and Technology(POSTECH), Ferrous Technology, Republic of Korea

**(GOMD-S1-SP009-2022) A two-point bending study of the failure characteristics of ion-exchanged glass fibers**T. C. Lewis<sup>\*1</sup>; R. Brow<sup>1</sup>; D. Thien<sup>1</sup>

1. Missouri University of Science & Technology, Materials Science and Engineering, USA

**(GOMD-S1-SP010-2022) Water as a flux in a hybrid coordination network glass**S. S. Sørensen<sup>\*1</sup>; X. Ren<sup>1</sup>; T. Du<sup>1</sup>; L. R. Jensen<sup>2</sup>; M. M. Smedskjaer<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Aalborg University, Department of Materials and Production, Denmark

**(GOMD-S1-SP011-2022) FTIR study on nanoceria created and extracted from a soluble sodium borate glass**K. S. Ranasinghe<sup>1</sup>; A. Vasquez<sup>\*1</sup>; R. Singh<sup>1</sup>

1. Kennesaw State University, Chemistry and Biochemistry, USA
2. Kennesaw State University, Physics, USA

**(GOMD-S1-SP012-2022) Characterization of sodium and calcium addition on aqueous interactions of binary borate glasses by vapor sorption**T. Yin<sup>\*1</sup>; W. C. Lepry<sup>1</sup>; M. T. Islam<sup>2</sup>; I. Ahmed<sup>2</sup>; P. Ouzilleau<sup>1</sup>; K. E. Waters<sup>1</sup>; S. N. Nazhat<sup>1</sup>

1. McGill University, Mining and Materials Engineering, Canada
2. University of Nottingham, Advanced Materials Research Group, United Kingdom

**(GOMD-S1-P013-2022) Incorporation of P<sub>2</sub>O<sub>5</sub>, MoO<sub>3</sub> and ZrO<sub>2</sub>-rich dismantling nuclear waste in an alkali-rich glass belonging to the SiO<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O-Li<sub>2</sub>O-CaO system**S. Achigar<sup>1</sup>; D. Caurant<sup>\*1</sup>; E. Régnier<sup>2</sup>; O. Majérus<sup>1</sup>; T. Charpentier<sup>3</sup>

1. Chimie Paristech CNRS, institut de recherche de Chimie Paris, France
2. CEA Marcoule, DEN, DE2D/SEVT/LDMC-Marcoule, France
3. NIMBE, CEA, CNRS, University Paris-Saclay, France



**(GOMD-S1-SP014-2022) Correlating Non-Synchrotron X-ray Techniques for Multiscale Imaging of Mo-containing Glasses**J. Bussey\*; M. Weber<sup>1</sup>; D. M. Cenda<sup>2</sup>; B. Faure<sup>2</sup>; S. Barton<sup>3</sup>; L. Moreau<sup>3</sup>; J. McCloy<sup>1</sup>

1. Washington State University, Institute of Materials Research, USA
2. Xenocs SAS, France
3. Xenocs Inc, USA
4. Washington State University, Department of Chemistry, USA

**(GOMD-S1-SP015-2022) Lithium-Iron Silicates as Simulations of High-Fe Nuclear Waste Glass**J. J. Erickson\*; J. McCloy<sup>1</sup>

1. Washington State University, Institute of Materials Research, USA

**(GOMD-S1-P016-2022) Impacts of Cr(III) and Cr(VI) concentrations on key high-level waste glass properties**V. Gervasio\*; S. Saslow<sup>1</sup>; D. Kim<sup>1</sup>; J. Vienna<sup>1</sup>

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA

**(GOMD-S1-SP017-2022) Impact of [Na<sub>2</sub>O]/[Al<sub>2</sub>O<sub>3</sub>] ratio and La<sub>2</sub>O<sub>3</sub> addition on the solubility of molybdenum oxide in aluminoborosilicate glasses**G. Dong\*; H. Kamat<sup>1</sup>; J. V. Hanna<sup>2</sup>; R. Youngman<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science Engineering, USA
2. University of Warwick, Department of Physics, United Kingdom
3. Corning Incorporated, Science and Technology Division, USA

**(GOMD-S1-SP018-2022) Preliminary Sintering Study for ZnO-Bi<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> Binder Glass**A. J. Lere-Adams\*; N. Stone-Weiss<sup>1</sup>; D. Bollinger<sup>1</sup>; J. McCloy<sup>1</sup>

1. Washington State University, Materials Science and Engineering Program, USA

**(GOMD-S1-SP019-2022) Scratch-induced Damage of Graphene-coated Silica Glass: A Molecular Dynamics Study**S. Sahoo\*; U. Tiwari<sup>1</sup>; R. R. Kaware<sup>2</sup>; S. Mannan<sup>2</sup>; N. N. Gosvami<sup>1</sup>; N. Krishnan<sup>2</sup>

1. Indian Institute of Technology Delhi, Materials Science and Engineering, India
2. Indian Institute of Technology Delhi, Department of Civil Engineering, India

**(GOMD-S1-SP020-2022) Laser-assisted processing of hermetic glass-to-metal seals**A. Read\*; R. Brow<sup>1</sup>; X. Wang<sup>1</sup>; D. Bristow<sup>1</sup>; D. Eichorst<sup>2</sup>

1. Missouri University of Science & Technology, USA
2. National Nuclear Security Administration Kansas City National Security, USA

**(GOMD-S1-SP021-2022) Effect of Glass Composition on the Laser-Induced Nucleation and Growth of Lithium Niobate Crystals in Lithium Niobosilicate Glass**K. J. Veenhuizen<sup>1</sup>; C. Barker<sup>2</sup>; J. Franklin\*; S. McAnany<sup>3</sup>; D. Nolan<sup>4</sup>; B. Aitken<sup>5</sup>; V. Dierolf<sup>1</sup>; H. Jain<sup>5</sup>

1. Lebanon Valley College, Physics, USA
2. Lehigh University, Physics, USA
3. II-VI Incorporated, USA
4. Corning Incorporated, USA
5. Lehigh University, Materials Science and Engineering, USA

**(GOMD-S1-SP022-2022) Photo-bleaching of Photo-Thermal-Refractive Glass**D. C. Lumpkin\*; R. Alvarez<sup>1</sup>; P. Shirshnev<sup>1</sup>; V. Smirnov<sup>2</sup>; L. Glebov<sup>1</sup>

1. University of Central Florida, CREOL, College of Optics and Photonics, USA
2. OptiGrate Corp, USA

**(GOMD-S1-SP023-2022) Mixed oxy-sulfide glassy solid electrolyte material: Structural characterization of 0.58Li<sub>2</sub>S + 0.42[(1-y)SiS<sub>2</sub> + yLiPO<sub>3</sub>]**P. J. Philipp\*; V. M. Torres<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, USA

**(GOMD-S1-SP024-2022) An Investigation of Haven's Ratio in Alkali Silicate Glasses Using Molecular Dynamics**S. S. White\*; E. Weber<sup>1</sup>; G. Kilpatrick<sup>1</sup>; C. B. Bragatto<sup>1</sup>

1. Coe College, Physics, USA

**(GOMD-S1-SP025-2022) Utilizing Electrical Impedance Spectroscopy (E.I.S.) to Observe In-Situ Phase Changes In Lithium Diborate Glass Undergoing Thermal Relaxation**W. Guthrie\*; C. B. Bragatto<sup>1</sup>

1. Coe College, Physics, USA

**(GOMD-S1-SP026-2022) Electrochemical characterization of a drawn thin-film glassy mixed oxy-sulfide-nitride phosphate electrolyte material for applications in solid-state batteries**M. Okkema\*; S. W. Martin<sup>1</sup>; M. P. Martin<sup>1</sup>

1. Iowa State University, Materials Science & Engineering, USA

**(GOMD-S1-SP027-2022) Lithium oxysilicate dopants in Li<sub>2</sub>S + SiS<sub>2</sub> glassy solid-state electrolyte systems**S. J. Leland\*; J. Wheaton<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, Materials Science and Engineering, USA

**(GOMD-S1-SP028-2022) Effect of crystallization on the electrical conductivity of vanado-tellurite glass doped with CuO, Cu<sub>2</sub>O, FeO and Fe<sub>2</sub>O<sub>3</sub>**M. Vacchi\*; C. Siligardi<sup>1</sup>; E. I. Cedillo-González<sup>1</sup>; M. Affatigato<sup>2</sup>

1. Università degli studi di Modena e Reggio Emilia, Italy
2. Coe College, Physics Department, USA

**(GOMD-S1-SP029-2022) Development of cathode materials for use with thin-film glassy solid electrolytes in solid-state batteries**W. Fekkether\*; J. Wheaton<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, Materials Science & Engineering, USA

**(GOMD-S1-P030-2022) Optimization of Antireflective Layers of Silicon Solar Cells: Comparative studies of the Efficiency between Single and Double Layer at the reference wavelength**

A. Diaw\*

1. Cheikh Anta Diop University, Physics, Senegal

**(GOMD-S1-SP031-2022) Materials Mitigation of Optical Nonlinearities for High Power Fiber Lasers**B. Meehan\*; T. Hawkins<sup>1</sup>; P. Dragic<sup>2</sup>; J. Ballato<sup>1</sup>

1. Clemson University, Materials Science and Engineering, USA
2. University of Illinois at Urbana-Champaign, Electrical and Computer Engineering, USA

**(GOMD-S1-SP032-2022) Yb-Doped Nanoparticle Silica Fibers for Anti-Stokes Fluorescence Cooling**M. A. Cahoon\*; B. Meehan<sup>1</sup>; T. Hawkins<sup>1</sup>; J. Ballato<sup>1</sup>; P. Dragic<sup>2</sup>; M. Engholm<sup>3</sup>; M. Dignonnet<sup>4</sup>

1. Clemson University, MSE, USA
2. University of Illinois at Urbana-Champaign, USA
3. Mid Sweden University, Sweden
4. Stanford University, USA

**(GOMD-S1-P033-2022) Novel Low Nonlinearity Optical Fibers Based on the Molten Core Method**M. Stone\*; A. Vonderhaar<sup>2</sup>; M. Cavillon<sup>2</sup>; T. Hawkins<sup>1</sup>; P. Dragic<sup>2</sup>; J. Ballato<sup>1</sup>

1. Clemson University, Materials Science and Engineering, USA
2. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA
3. University of Paris-Saclay, France

**(GOMD-S1-SP034-2022) North American Summer School on Photonic Materials (NASSPM): Student retrospectives towards their graduate education and future careers**E. J. Musterman\*; C. Barker<sup>2</sup>

1. Lehigh University, Materials Science and Engineering, USA
2. Lehigh University, Physics, USA

**(GOMD-S1-P035-2022) Mid-IR absorption in photo-thermo-refractive glass**P. Shirshnev\*; L. Glebov<sup>1</sup>

1. University of Central Florida, CREOL, USA

**(GOMD-S1-P036-2022) Modeling the Formation of foam Glass**T. Keith\*; G. Craft<sup>1</sup>; M. Laugen<sup>1</sup>; C. L. Trivelpiece<sup>2</sup>; C. Wilkinson<sup>1</sup>

1. GlassWRX, Department of Research & Development, USA
2. Savannah River National Lab, USA

## Tuesday, May 24, 2022

### Award Lectures

#### George W. Morey Award Lecture

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

**8:00 AM**

#### Introduction

**8:10 AM**

#### (GOMD-AW-002-2022) Optical Fiber meets the Periodic Table: The past, present, and future of the molten core method

J. Ballato\*<sup>1</sup>

1. Clemson University, Materials Science and Engineering, USA

**8:50 AM**

#### Award Presentation

### S1: Fundamentals of the Glassy State

#### Structure of Glasses I

Room: Columbia (Second floor)

Session Chair: Thibault Charpentier, CEA

**9:20 AM**

#### (GOMD-S1-017-2022) Extent of structural disorder in glasses and transparent ceramic from advanced solid-state NMR spectroscopy (Invited)

F. Fayon\*<sup>1</sup>; A. Ridouard<sup>1</sup>; L. Piveteau<sup>1</sup>; C. Genevois<sup>1</sup>; M. Pitcher<sup>1</sup>; M. Allix<sup>1</sup>; D. Massiot<sup>1</sup>

1. CNRS, CEMHTI, France

**9:50 AM**

#### (GOMD-S1-018-2022) Effect of adding Al<sub>2</sub>O<sub>3</sub> on the structure and properties of LaB<sub>3</sub>O<sub>6</sub> glass

D. Caurant\*<sup>1</sup>; E. Chesneau<sup>2</sup>; T. Charpentier<sup>3</sup>; O. Majérus<sup>1</sup>

1. Chimie Paristech CNRS, institut de recherche de Chimie Paris, France
2. CNRS, CEMTHI UPR 3079, France
3. NIMBE CEA Paris-Saclay, CEA CNRS Université Paris-Saclay, France

**10:10 AM**

#### (GOMD-S1-019-2022) Structure and its effect on the crystallization behavior of mold flux glasses in the system CaO-SiO<sub>2</sub>-CaF<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O: Results from Multinuclear NMR Spectroscopy

T. Yeo<sup>1</sup>; J. Cho<sup>2</sup>; S. Sen\*<sup>1</sup>

1. University of California, Davis, Department of Material Science and Engineering, USA
2. Pohang University of Science and Technology, Graduate Institute of Ferrous & Energy Materials Technology, Republic of Korea

**10:30 AM**

#### (GOMD-S1-020-2022) Insight into the partitioning and clustering mechanism of rare earth cations in alkali aluminoborosilicate glasses

H. Kamat\*<sup>1</sup>; F. Wang<sup>1</sup>; K. E. Barnsley<sup>2</sup>; J. V. Hanna<sup>2</sup>; A. Tyryshkin<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers, The State University of New Jersey, Materials Science and Engineering, USA
2. University of Warwick, Department of Physics, United Kingdom
3. Rutgers, The State University of New Jersey, Marine and Coastal Sciences, USA

**10:50 AM**

#### (GOMD-S1-021-2022) Octahedral oxide glass networks at ambient pressure: Structure of neodymium titanate glass

S. K. Wilke\*<sup>1</sup>; O. L. Alderman<sup>1</sup>; C. J. Benmore<sup>2</sup>; J. Neuefeind<sup>3</sup>; R. Weber<sup>1</sup>

1. Materials Development, Inc., USA
2. Argonne National Lab, X-ray Science Division, Advanced Photon Source, USA
3. Oak Ridge National Lab, Neutron Science Division, Spallation Neutron Source, USA
4. Rutherford Appleton Laboratory, ISIS Neutron and Muon Source, United Kingdom

### Topology and Rigidity

Room: Constellation E (Second floor)

Session Chairs: Mathieu Bauchy, University of California, Los Angeles; Morten Smedskjaer, Aalborg University

**9:20 AM**

#### (GOMD-S1-022-2022) Low-Dimensional Representation of the Short- and Medium-Range Structure of Glassy Materials (Invited)

T. J. Hardin\*<sup>1</sup>; M. Wilson<sup>1</sup>; M. Chandross<sup>1</sup>; M. Shields<sup>3</sup>; M. L. Falk<sup>2</sup>

1. Sandia National Laboratories, Computational Materials and Data Science, USA
2. Johns Hopkins University, Materials Science and Engineering, USA
3. Johns Hopkins University, Civil and Systems Engineering, USA

**9:50 AM**

#### (GOMD-S1-023-2022) Molecular origin of the super-strong behavior of melt dynamics in the Intermediate Phase of chalcogenide glasses

B. S. Almutairi\*<sup>1</sup>; R. Chbeir<sup>2</sup>; A. Welton<sup>2</sup>; M. Burger<sup>2</sup>; S. Chakravarty<sup>3</sup>; P. Boolchand<sup>2</sup>

1. Princess Nourah Bint Abdulrahman University, Physics, Saudi Arabia
2. University of Cincinnati, Electrical Engineering and Computer Science, USA
3. University of Cincinnati, Mechanical and Materials Engineering, USA

**10:10 AM**

#### (GOMD-S1-024-2022) Structure-property relationship in covalent network glasses: Relative influence of three structural features

P. Lucas\*<sup>1</sup>

1. Univ of Arizona, USA

**10:30 AM**

#### (GOMD-S1-025-2022) Learning topology of disordered materials through graph neural network

N. Krishnan\*<sup>1</sup>; V. Bihani<sup>1</sup>; S. Manchanda<sup>1</sup>; S. Ranu<sup>1</sup>

1. Indian Institute of Technology Delhi, Civil Engineering, India

**10:50 AM**

#### (GOMD-S1-026-2022) Understanding diffraction patterns and topologies of disordered materials (Invited)

Y. Onodera\*<sup>1</sup>; S. Kohara<sup>2</sup>

1. Kyoto University, Institute for Integrated Radiation and Nuclear Science, Japan
2. National Institute for Materials Science (NIMS), Japan

**11:20 AM**

#### (GOMD-S1-027-2022) Glass Irradiation: Impact on Structure and Mechanical Properties

M. M. Smedskjaer\*<sup>1</sup>; T. Du<sup>1</sup>; X. Ren<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

**11:40 AM**

#### (GOMD-S1-028-2022) A More Suitable Way to Calculate Glass Packing Fraction and its Application for Young's Modulus Prediction (Invited)

Y. Shi\*<sup>1</sup>; A. Tandia<sup>1</sup>; S. Elliott<sup>2</sup>; M. Bauchy<sup>3</sup>

1. Corning Incorporated, USA
2. University of Oxford, United Kingdom
3. University of California, Los Angeles, USA

**12:10 PM**

#### (GOMD-S1-029-2022) Decoding the Topological Origin of the Thermal Expansion of Glasses

Q. Zhou<sup>1</sup>; M. Bauchy\*<sup>1</sup>

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

## **S2: Glass and Interactions with Its Environment: Fundamentals and Applications**

### **Dissolution and Interfacial Reactions III: Modeling Glass Dissolution and Glass Interaction with Various Environments**

Room: Constellation C/D (Second floor)

Session Chairs: Joseph Ryan, Pacific Northwest National Lab; Nicholas Stone-Weiss, Corning Incorporated

**9:20 AM**

#### **(GOMD-S2-025-2022) Advances of atomistic computer simulations in understanding glass-water interactions (Invited)**

T. S. Mahadevan<sup>\*</sup>; J. Du<sup>1</sup>

1. University of North Texas, Materials Science and Engg, USA

**9:50 AM**

#### **(GOMD-S2-026-2022) Quantitative Structural Property Relationship analysis of dissolution rate of aluminosilicate and borosilicate glasses**

J. Du<sup>\*</sup>; X. Lu<sup>2</sup>; J. Vienna<sup>3</sup>; J. V. Ryan<sup>2</sup>; M. Bauchy<sup>3</sup>; J. Delaue<sup>4</sup>; S. Gin<sup>4</sup>

1. University of North Texas, Materials Science and Engineering, USA
2. Pacific Northwest National Laboratory, USA
3. UCLA, USA
4. CEA, France

**10:10 AM**

#### **(GOMD-S2-027-2022) Predictive Modeling of Stage III Leach Rate Resumption in Nuclear Waste Glasses**

I. S. Muller<sup>\*</sup>; K. Gilbo<sup>1</sup>; I. Pegg<sup>1</sup>

1. The Catholic University of America, Vitreous State Laboratory, USA

**10:30 AM**

#### **(GOMD-S2-028-2022) Dissolution behavior and kinetics of alkali/alkaline-earth aluminoborosilicate glasses in hyperalkaline media: Impact of high ionic field strength non-framework cations**

Q. Qin<sup>\*</sup>; N. Stone-Weiss<sup>1</sup>; Z. Zhao<sup>2</sup>; P. Mukherjee<sup>2</sup>; J. Ren<sup>2</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Key Laboratory of Materials for High-Power Laser, China
3. Michigan Technological University, Materials Science and Engineering, USA

**10:50 AM**

#### **(GOMD-S2-029-2022) Predicting mineral wool fibers dissolution in biological environments by in vitro tests and thermodynamics**

N. Drnovsek<sup>\*</sup>; U. Kovacic<sup>1</sup>; D. Trivunecvic<sup>2</sup>; M. Debeljak<sup>1</sup>; E. Pezennec<sup>1</sup>; P. Kiefer<sup>1</sup>; D. Laurent<sup>1</sup>; J. DeMott<sup>1</sup>; M. Strlic<sup>2</sup>; R. Conrad<sup>3</sup>

1. Knauf Insulation, Slovenia
2. Faculty of Chemistry and Chemical Technology, Slovenia
3. UniglassAC GmbH, Germany

**11:10 AM**

#### **(GOMD-S2-030-2022) Aging Effects on the Failure Characteristics of Ion Exchanged Alkali Aluminosilicate Glass**

R. Grodsky<sup>\*</sup>; R. Brow<sup>2</sup>

1. Honeywell FM&T, USA
2. Missouri University of Science & Technology, Materials Science & Eng, USA

**11:30 AM**

#### **(GOMD-S2-031-2022) Quantifying residual stress during case II diffusion of water in Na<sub>2</sub>O-3SiO<sub>2</sub> glass**

B. D. Hausmann<sup>\*</sup>; M. Tomozawa<sup>1</sup>

1. Rensselaer Polytechnic Institute, Materials Science & Engineering, USA

## **Nuclear Waste Immobilization I**

Room: Frederick (Second floor)

Session Chair: John McCloy, Washington State University

**9:20 AM**

#### **(GOMD-S2-032-2022) Effect of melter feed composition and properties on the rate of melting during vitrification of nuclear waste (Invited)**

R. Pokorny<sup>\*</sup>; J. Klouzek<sup>1</sup>; M. Vernerova<sup>1</sup>; P. Ferkl<sup>2</sup>; J. Marcial<sup>2</sup>; S. Lee<sup>2</sup>; P. Hrma<sup>2</sup>; A. A. Kruger<sup>3</sup>

1. University of Chemistry and Technology Prague, Czechia
2. Pacific Northwest National Lab, USA
3. US Department of Energy, Office of River Protection, USA

**9:50 AM**

#### **(GOMD-S2-033-2022) Low Activity Waste Glass Optimization with Machine Learning**

X. Lu<sup>\*</sup>; J. Vienna<sup>1</sup>

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA

**10:10 AM**

#### **(GOMD-S2-034-2022) Understanding the Effects of Anions on Sulfate Retention in Low Active Waste Glasses**

N. J. Smith-Gray<sup>\*</sup>; N. Stone-Weiss<sup>1</sup>; J. M. Loneragan<sup>2</sup>; J. McCloy<sup>1</sup>

1. Washington State University, Materials Science and Engineering, USA
2. Pacific Northwest National Lab, USA

**10:30 AM**

#### **(GOMD-S2-035-2022) Effect of iron and chromium on sulfur solubility in alkali borosilicate glasses**

X. Xu<sup>\*</sup>; S. Kamali<sup>2</sup>; A. Pedone<sup>2</sup>; A. Tyryshkin<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, MSE, USA
2. Tennessee Space Institute, USA
3. University of Modena and Reggio Emilia, Italy
4. Rutgers University, USA

**10:50 AM**

#### **(GOMD-S2-036-2022) Re Volatilization during Nuclear Waste Vitrification: The Salt Effects**

C. Niu<sup>\*</sup>; L. Peng<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State Key Laboratory of Silicate Materials for Architectures, China

**11:10 AM**

#### **(GOMD-S2-037-2022) Development of Phosphate Glass Waste Forms To Immobilize Salt Waste Stream**

M. Tang<sup>\*</sup>

1. Clemson University, Department of Materials Science & Engineering, USA

**11:30 AM**

#### **(GOMD-S2-038-2022) Dechlorination and Vitrification of Electrochemical Processing Salt Simulant**

Y. Dong<sup>\*</sup>; Z. Jia<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State Key Laboratory of Silicate Materials for Architectures (SMART), China

**11:50 AM**

#### **(GOMD-S2-039-2022) Dependence of Monofrax™ K-3 refractory corrosion on the melt chemistry**

X. Xu<sup>\*</sup>; R. Saini<sup>2</sup>; K. Akdoğan<sup>1</sup>; A. Goel<sup>1</sup>

1. Rutgers University, MSE, USA
2. Akal University, India



**S4: Glass Technology and Cross-Cutting Topics****Batch to Glass Conversion**

Room: Constellation F (Second floor)

Session Chairs: Jonathan Icenhower, Corning Incorporated;  
Irene Peterson, Corning Incorporated**9:20 AM****(GOMD-S4-014-2022) In-situ visual observations of glass melting processes for nuclear waste vitrification (Invited)**J. Marcial<sup>\*2</sup>; R. Pokorny<sup>1</sup>; J. Klouzek<sup>1</sup>; M. Vernerova<sup>1</sup>; P. Ferkl<sup>2</sup>; P. Hrna<sup>3</sup>; A. A. Kruger<sup>4</sup>

1. University of Chemistry and Technology, Prague, Laboratory of Inorganic Materials, Czechia
2. Pacific Northwest National Lab, USA
3. AttainX, USA
4. DOE Office of River Protection, USA

**9:50 AM****(GOMD-S4-015-2022) Batch-to-glass conversion kinetics in joule-heated melters (Invited)**P. Ferkl<sup>\*1</sup>; P. Hrna<sup>2</sup>; A. Abboud<sup>2</sup>; D. P. Guillen<sup>3</sup>; M. Vernerová<sup>4</sup>; J. Klouzek<sup>4</sup>; J. Marcial<sup>1</sup>; M. Hall<sup>1</sup>; A. A. Kruger<sup>2</sup>; R. Pokorny<sup>4</sup>

1. PNNL, USA
2. AttainX, USA
3. Idaho National Lab, USA
4. UCT Prague, Czechia
5. US DOE, USA

**10:20 AM****(GOMD-S4-016-2022) The Effect of Glass Surface Fluidity on Melting Reactions (Invited)**D. R. Swiler<sup>\*1</sup>

1. O-I, R&D, USA

**10:50 AM****(GOMD-S4-017-2022) Glass melting and phase separation: Modeling and simulation approaches (Invited)**S. Schuller<sup>\*1</sup>; E. Sauvage<sup>1</sup>; K. Paraiso<sup>2</sup>; A. Cartalade<sup>3</sup>; W. Verdier<sup>3</sup>; S. Gossé<sup>4</sup>; R. le tellier<sup>5</sup>

1. CEA, ISEC/DE2D, France
2. Saint-Gobain Research Provence, France
3. CEA, ISAS/DM2S, France
4. CEA, ISAS, France
5. CEA, IRESNE/DTN, France

**11:20 AM****(GOMD-S4-018-2022) Oxidize Sulfate Fining in Borosilicate Glasses**S. M. Jarvis<sup>\*1</sup>

1. Corning Incorporated, USA

**11:40 AM****(GOMD-S4-019-2022) Nanoparticle Formation During Production of Copper Borate Glass in Stainless Steel Crucibles**P. N. DeMaere<sup>\*1</sup>; W. Wall<sup>2</sup>; S. Adab<sup>2</sup>; Y. Boluk<sup>1</sup>; C. Calahoo<sup>1</sup>

1. University of Alberta, Civil and Environmental Engineering, Canada
2. Genics Inc., Canada

**Award Lectures****Norbert J. Kreidl Award for Young Scholars**

Room: Constellation C/D (Second floor)

Session Chair: Charmayne Lonergan, Pacific Northwest National Lab

**12:15 PM****Introduction****12:25 PM****(GOMD-AW-003-2022) Synthesis, structure and properties of pure TeO<sub>2</sub> glass, binary and ternary tellurite glasses**N. Tagiara<sup>\*1</sup>

1. National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Greece

**S1: Fundamentals of the Glassy State****Glass Formation and Structural Relaxation I**

Room: Constellation E (Second floor)

Session Chairs: Sabyasachi Sen, University of California, Davis; Collin Wilkinson, Pennsylvania State University

**1:20 PM****(GOMD-S1-030-2022) Glasses Prepared by Physical Vapor Deposition (Invited)**J. Gabriel<sup>1</sup>; E. Thoms<sup>1</sup>; R. Richert<sup>\*1</sup>

1. Arizona State University, School of Molecular Sciences, USA

**1:50 PM****(GOMD-S1-031-2022) Influence of the modifier type on the surface properties of alkali silicate glasses (Invited)**W. Kob<sup>\*1</sup>; Z. Zhang<sup>2</sup>; S. Ispas<sup>1</sup>

1. University of Montpellier, France
2. Xi'an Jiaotong University, State Key Laboratory for Mechanical Behavior of Materials, China

**2:20 PM****(GOMD-S1-032-2022) Mixed-Alkali Effect on the Fragility and Viscoelasticity of Metaphosphate Glass Forming Liquids**T. Yeo<sup>\*1</sup>; S. Sen<sup>1</sup>

1. University of California, Davis, Materials Science and Engineering, USA

**2:40 PM****(GOMD-S1-033-2022) The glass formation boundary in aluminosilicates**H. Lee<sup>\*1</sup>; W. M. Carty<sup>1</sup>

1. Alfred University, New York State College of Ceramics, USA

**3:00 PM****(GOMD-S1-034-2022) Evidence of Ionic Relaxation in the Dynamic Light Scattering of Sodium Borate Melts**D. Sidebottom<sup>\*1</sup>; H. Uppala<sup>1</sup>

1. Creighton University, Physics, USA

**3:20 PM****Break****Glass Formation and Structural Relaxation II**

Room: Constellation E (Second floor)

Session Chair: Sabyasachi Sen, University of California, Davis

**3:40 PM****(GOMD-S1-035-2022) Regularities in structural development of As- and Ge-based chalcogenide glasses (Invited)**R. Golovchak<sup>\*1</sup>

1. Austin Peay State University, Physics and Astronomy, USA

**4:10 PM****(GOMD-S1-036-2022) Structural relaxation in chalcogenide glasses (Invited)**J. Malek<sup>\*1</sup>

1. University of Pardubice, Department of Physical Chemistry, Czechia

**4:40 PM****(GOMD-S1-037-2022) Revisiting the Adam-Gibbs Equation through Energy Landscape Modeling**C. Wilkinson<sup>\*1</sup>; J. C. Mauro<sup>2</sup>

1. GlassWRX, USA
2. Pennsylvania State University, Department of Materials Science and Engineering, USA

**5:00 PM****(GOMD-S1-038-2022) Non-Arrhenius Viscous Behavior and the Rate of Change of the Energy Landscape Topography**M. C. Beg<sup>\*1</sup>; J. Kieffer<sup>1</sup>

1. University Of Michigan, USA

**Structure of Glasses II**

Room: Columbia (Second floor)

Session Chair: Oliver Alderman, STFC

**1:20 PM****(GOMD-S1-039-2022) Effect of the type of modifier on structure and properties of borosilicate glasses – a spectroscopic study (Invited)**D. Möncke\*<sup>1</sup>

1. Alfred University, Inamori School of Engineering at the NYSCC, USA

**1:50 PM****(GOMD-S1-040-2022) Structural study of alkaline earth aluminosilicate glasses by vibrational spectroscopy**J. L. Hunt\*<sup>1</sup>; R. Youngman<sup>2</sup>; A. Herrmann<sup>4</sup>; E. I. Kamitsos<sup>3</sup>; D. Möncke<sup>1</sup>

1. Alfred University, USA
2. Corning Incorporated, USA
3. National Hellenic Research Foundation, Greece
4. Technical University Ilmenau, Germany

**2:10 PM****(GOMD-S1-041-2022) Structure and Crystallization in TiO<sub>2</sub>-containing Nepheline Glasses**J. McCloy\*<sup>1</sup>; E. T. Nienhuis<sup>2</sup>; N. J. Smith-Gray<sup>1</sup>; J. Marcial<sup>2</sup>; N. C. Hyatt<sup>3</sup>; L. Mottram<sup>3</sup>; M. C. Stennett<sup>3</sup>; C. Le Losq<sup>4</sup>; D. R. Neuville<sup>4</sup>; Y. Zhang<sup>5</sup>; A. Goel<sup>3</sup>

1. Washington State University, School of Mechanical and Materials Engineering, USA
2. Pacific Northwest National Lab, USA
3. University of Sheffield, United Kingdom
4. Institut de Physique du Globe de Paris (IPGP), France
5. Rutgers University, USA

**2:30 PM****(GOMD-S1-042-2022) Experimental Method to Quantify the Ring Size Distribution in Silicate Glasses and Its Simulation Validation**Y. Shi\*<sup>1</sup>; Q. Zhou<sup>2</sup>; J. Neufeind<sup>3</sup>; M. Bauchy<sup>2</sup>

1. Corning Incorporated, Characterization Science, USA
2. University of California, Los Angeles, USA
3. Oak Ridge National Lab, Neutron Scattering Division, USA

**2:50 PM****(GOMD-S1-043-2022) Structure, viscosity and mixing in Li<sub>2</sub>O/MO (M=Mg, Ca, Sr, Ba) silicate glasses and melts**D. R. Neuville\*<sup>1</sup>

1. IPGP, géomatériaux, France

**3:10 PM****Break****Structure of Glasses III**

Room: Columbia (Second floor)

Session Chair: Franck Fayon, CNRS

**3:40 PM****(GOMD-S1-044-2022) Structure, and Mechanical Properties of Glassy Sulfide Solid Electrolytes (Invited)**K. Ohara\*<sup>1</sup>; A. Sakuda<sup>2</sup>; A. Hayashi<sup>2</sup>

1. Japan Synchrotron Radiation Research Institute, Diffraction and Scattering Division, Japan
2. Osaka Prefecture University, Graduate School of Engineering, Japan

**4:10 PM****(GOMD-S1-045-2022) Observation of a Reentrant Liquid-Liquid transition in an Arsenic Sulfide Glass-forming Liquid**B. Yuan\*<sup>1</sup>; S. Sen<sup>1</sup>

1. University of California, Davis, Materials Science and Engineering, USA

**4:30 PM****(GOMD-S1-046-2022) Investigation of the Properties of Fragile Metal Oxide Liquids**R. Weber\*<sup>1</sup>; S. K. Wilke<sup>1</sup>; C. J. Benmore<sup>2</sup>; M. SanSoucie<sup>3</sup>; V. Menon<sup>3</sup>; J. Rafferty<sup>3</sup>; S. Kohara<sup>4</sup>; H. Oda<sup>4</sup>; C. Koyama<sup>4</sup>; T. Ishikawa<sup>4</sup>

1. MDI, USA
2. Argonne National Lab, USA
3. NASA, USA
4. National Institute for Materials Science (NIMS), Japan
5. JAXA, Japan

**4:50 PM****(GOMD-S1-047-2022) Boron coordination change and the fragility maximum in glass-forming liquid lithium borates**O. L. Alderman\*<sup>1</sup>; C. J. Benmore<sup>2</sup>; S. Feller<sup>3</sup>; R. Weber<sup>4</sup>

1. STFC, ISIS Neutron and Muon Source, United Kingdom
2. Argonne National Lab, X-ray Science Division, USA
3. Coe College, USA
4. Materials Development, Inc., USA

**S2: Glass and Interactions with Its Environment: Fundamentals and Applications****Nuclear Waste Immobilization II**

Room: Frederick (Second floor)

Session Chair: Daniel Caurant, Chimie Paristech CNRS

**1:20 PM****(GOMD-S2-040-2022) Multivariate Analysis: An essential for studying complex glasses**I. Sargin\*<sup>1</sup>; J. McCloy<sup>2</sup>; S. Beckman<sup>2</sup>

1. Middle East Technical University, Metallurgical and Materials Engineering, Turkey
2. Washington State University, School of Mechanical and Materials Engineering, USA

**1:40 PM****(GOMD-S2-041-2022) Impact of mixed network former effect on spinel crystallization in high-level nuclear waste glasses**N. Balasubramanya\*<sup>1</sup>; P. Florian<sup>2</sup>; A. Scrimshire<sup>3</sup>; P. A. Bingham<sup>3</sup>; M. Ahmadzadeh<sup>4</sup>; J. McCloy<sup>5</sup>; M. I. Tuheen<sup>2</sup>; J. Du<sup>2</sup>; S. Kamali<sup>6</sup>; A. Goel<sup>1</sup>

1. Rutgers-The State University of New Jersey, Materials Science and Engineering, USA
2. CNRS, CEMHTI, France
3. Sheffield Hallam University, Materials and Engineering Research Institute, United Kingdom
4. Washington State University, School of Mechanical and Materials Engineering, USA
5. University of North Texas, Department of Materials Science and Engineering, USA
6. Middle Tennessee State University, Department of Physics and Astronomy, USA

**2:00 PM****(GOMD-S2-042-2022) Impact of non-framework cation mixing on the structure and crystallization behavior of model high-level nuclear waste glasses**N. Balasubramanya\*<sup>1</sup>; Z. Sun<sup>1</sup>; M. Ahmadzadeh<sup>2</sup>; S. Kamali<sup>3</sup>; D. R. Neuville<sup>4</sup>; J. McCloy<sup>2</sup>; A. Goel<sup>1</sup>

1. Rutgers-The State University of New Jersey, Materials Science and Engineering, USA
2. Washington State University, School of Mechanical and Materials Engineering, USA
3. Middle Tennessee State University, Department of Physics and Astronomy, USA
4. CNRS, IPGP, France

**2:20 PM****(GOMD-S2-043-2022) Insights into the of iron and phosphorus induced structural disorder in sodium aluminoborosilicate glasses and its impact on their melt rheology and crystallization behavior**Y. Zhang\*<sup>1</sup>; N. Balasubramanya<sup>1</sup>; N. Stone-Weiss<sup>2</sup>; S. Kamali<sup>4</sup>; R. Youngman<sup>3</sup>; P. Florian<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Corning Incorporated, USA
3. CNRS, France
4. University of Tennessee Space Institute, USA

**2:40 PM****(GOMD-S2-044-2022) Does CaO suppress nepheline crystallization in high-level waste glasses?**Y. Zhang\*<sup>1</sup>; R. Youngman<sup>2</sup>; A. Pedone<sup>3</sup>; M. Bertani<sup>3</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Corning Incorporated, USA
3. University of Reggio Emilia, Italy

**3:00 PM****(GOMD-S2-045-2022) Diopside Crystallization in A Simulated HLW Glass**R. Jia\*<sup>1</sup>; C. Niu<sup>1</sup>; Z. Jia<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State key Laboratory of Silicate Materials for Architectures, China

**3:20 PM****Break**

\*Denotes Presenter

**3:40 PM****(GOMD-S2-046-2022) Chemical durability assessment of enhanced low-activity waste glasses through EPA method 1313**J. Marcial<sup>\*</sup>; J. Neeway<sup>1</sup>; C. Pearce<sup>1</sup>; J. Vienna<sup>1</sup>; L. Nava-Farias<sup>1</sup>; C. L. Thorpe<sup>2</sup>; C. L. Corkhill<sup>2</sup>; R. J. Hand<sup>2</sup>; D. Kosson<sup>3</sup>; R. Delapp<sup>3</sup>; A. A. Kruger<sup>4</sup>

1. Pacific Northwest National Lab, USA
2. University of Sheffield, United Kingdom
3. Vanderbilt University, USA
4. U.S. DOE Office of River Protection, USA

**4:00 PM****(GOMD-S2-047-2022) Structural Integrity of Residual (SIR) Glass Model to Augment Nuclear Waste Glass Design**J. Amoroso<sup>\*</sup>; D. L. McClane<sup>1</sup>; M. Hsieh<sup>1</sup>; A. A. Kruger<sup>2</sup>

1. Savannah River National Laboratory, USA
2. US Department of Energy, Office of River Protection, USA

**4:20 PM****(GOMD-S2-048-2022) Characterisation of vitrified Scottish hillfort materials from a nuclear-waste glass analogue perspective**J. T. Mansfield<sup>\*</sup>; C. L. Corkhill<sup>1</sup>; M. T. Harrison<sup>2</sup>; R. J. Hand<sup>1</sup>

1. The University of Sheffield, Department of Materials Science and Engineering, United Kingdom
2. National Nuclear Laboratory, United Kingdom

**4:40 PM****(GOMD-S2-049-2022) Vitrification of Radioactive Glass Fiber from Nuclear Facilities**G. Fang<sup>\*</sup>; X. Zhao<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State Key Laboratory of Silicate Materials for Architectures, China

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Charge and Energy Transport in Disordered Materials**

Room: Constellation F (Second floor)

Session Chair: Caio Bragatto, Coe College

**1:20 PM****(GOMD-S3-021-2022) Improved storage of electric power (Invited)**M. Braga<sup>\*</sup>

1. University of Porto, Engineering Physics Department, Engineering Faculty, Portugal

**1:50 PM****(GOMD-S3-022-2022) Elucidating Li's Role in the Architecture of Active Li-ion Cells with Neutron Depth Profiling**J. L. Weaver<sup>\*</sup>

1. National Institute of Standards and Technology, Material Measurement Laboratory, USA

**2:10 PM****(GOMD-S3-023-2022) Effects of oxy-silicate dopants in Li<sub>2</sub>S – SiS<sub>2</sub> based glassy solid-state electrolyte systems**J. Wheaton<sup>\*</sup>; S. Leland<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, Materials Science and Engineering, USA

**2:30 PM****(GOMD-S3-025-2022) Preparation and characterization of new Li-Si-P-S-O-N glasses: Comparison of the effects of different starting materials**V. M. Torres<sup>\*</sup>; P. J. Philipp<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, Materials Science and Engineering, USA

**2:50 PM****(GOMD-S3-027-2022) Correlating thermal conductivity of oxide glasses with modal characteristics and network topology**S. S. Sørensen<sup>\*</sup>; P. P. Cielecki<sup>1</sup>; H. Johra<sup>2</sup>; M. Bockowski<sup>2</sup>; E. Skovsen<sup>4</sup>; M. M. Smedskjaer<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Institute of High-Pressure Physics Polish Academy of Sciences, Poland
3. Aalborg University, Department of the Built Environment, Denmark
4. Aalborg University, Department of Materials and Production, Denmark

**Wednesday, May 25, 2022****Award Lectures****Varshneya Glass Science Lecture**

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

**8:00 AM****Introduction****8:10 AM****(GOMD-AW-004-2022) Chalcogenide optical materials: A 'coming of age' story**K. A. Richardson<sup>\*</sup>

1. University of Central Florida, College of Optics and Photonics, Dept. of Materials Science and Eng., USA

**8:50 AM****Award Presentation****S1: Fundamentals of the Glassy State****Improved Methods for Glass Structure Determination**

Room: Constellation F (Second floor)

Session Chair: Sushmit Goyal, Corning Incorporated

**9:20 AM****(GOMD-S1-048-2022) Solving structural puzzles in amorphous materials by combining first-principles and machine learning molecular dynamics (Invited)**G. Ori<sup>\*</sup>

1. Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), CNRS | Univ. Strasbourg, France

**9:50 AM****(GOMD-S1-049-2022) A NMR-Driven Reverse Monte Carlo Study of Sodium Borate Glasses**T. Charpentier<sup>\*</sup>; E. Chesneau<sup>2</sup>; L. Cormier<sup>1</sup>; G. Tricot<sup>2</sup>

1. Sorbonne Université, IMPMC, France
2. Université de Lille, LASIR, France
3. Université Paris-Saclay, CEA, IRAMIS/NIMBE, France

**10:10 AM****(GOMD-S1-050-2022) Predicting the Dynamics of Atoms in Glass-Forming Liquids by a Surrogate Machine-Learned Simulator**H. Liu<sup>1</sup>; M. Bauchy<sup>\*</sup>

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

**10:30 AM****(GOMD-S1-051-2022) Improved empirical force field for molecular dynamics simulations of oxide glasses**M. Bertani<sup>\*</sup>; A. Pedone<sup>1</sup>; M. Menziani<sup>1</sup>

1. University of Modena and Reggio Emilia, Department of Chemical and Geological Sciences, Italy

**10:50 AM****(GOMD-S1-052-2022) Development of a molecular dynamics framework to study the kinetics of thermal poling: Application to sodium silicate glasses**P. Ammu<sup>\*</sup>; M. Reveil<sup>1</sup>; C. McLaren<sup>1</sup>; N. J. Smith<sup>1</sup>; A. Tandia<sup>1</sup>

1. Corning Incorporated, USA

**11:10 AM****(GOMD-S1-053-2022) Atomic Structure of Amorphous Oxide Thin Films by Fitting to X-ray and Electron Diffraction Datasets**K. Prasai<sup>\*</sup>; K. Lee<sup>2</sup>; J. Jiang<sup>3</sup>; H. Cheng<sup>3</sup>; R. Bassiri<sup>1</sup>; M. Fejer<sup>1</sup>

1. Stanford University, Applied Physics, USA
2. Sungkyunkwan University, Physics, Republic of Korea
3. University of Florida, Physics, USA



**11:30 AM****(GOMD-S1-054-2022) Structures of niobium-containing silicate glasses from MD simulations with newly developed niobium potential**W. Sun<sup>\*1</sup>; K. J. Veenhuizen<sup>2</sup>; J. Marsh<sup>2</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>1</sup>

1. Lehigh University, Material Science and Engineering, USA
2. Lebanon Valley College, Department of Physics, USA
3. Lehigh University, Department of Physics, USA

**11:50 AM****(GOMD-S1-055-2022) Molecular dynamics simulation of tellurite glasses**A. Jan<sup>\*1</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, India

**Non-oxide Glasses and Glass-ceramics I**

Room: Constellation E (Second floor)

Session Chair: Pierre Lucas, Univ of Arizona

**9:20 AM****(GOMD-S1-056-2022) Progress in Hybrid Glass Formation, Characterization and Properties (Invited)**T. Bennett<sup>\*1</sup>

1. University of Cambridge, United Kingdom

**9:50 AM****(GOMD-S1-057-2022) Solution-Processed Telluride Glass for Far-Infrared Applications (Invited)**L. Moghimi<sup>\*2</sup>; P. Wondrak<sup>1</sup>; P. Lucas<sup>1</sup>

1. Univ of Arizona, USA
2. Stanford University, USA

**10:20 AM****(GOMD-S1-058-2022) Vitrification of organic semiconductor mixtures with ultralow fragility (Invited)**C. Müller<sup>\*1</sup>

1. Chalmers University of Technology, Sweden

**10:50 AM****(GOMD-S1-059-2022) High refractive index IR lenses based on chalcogenide glasses molded by Spark Plasma Sintering**V. Reux<sup>\*1</sup>; L. Calvez<sup>1</sup>; X. Zhang<sup>1</sup>

1. ISCR, France

**11:10 AM****(GOMD-S1-060-2022) Crystallization in glasses in the Ga-Sb-Se ternary system**L. Verger<sup>\*1</sup>; V. Nazabal<sup>1</sup>; D. Le Coq<sup>1</sup>; L. Calvez<sup>1</sup>

1. Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) – UMR 6226, France

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Laser Interactions with Glasses**

Room: Frederick (Second floor)

Session Chair: Casey Schwarz, Ursinus College

**9:20 AM****(GOMD-S3-028-2022) Laser-induced crystallization in glass: The influence of laser specific properties (Invited)**V. Dierolf<sup>\*1</sup>; C. Au-Yeung<sup>1</sup>; E. J. Musterman<sup>2</sup>; H. Jain<sup>2</sup>

1. Lehigh University, Physics, USA
2. Lehigh University, Materials Science and Engineering, USA

**9:50 AM****(GOMD-S3-029-2022) Orientability of nanocrystals induced by a laser in oxide glasses (Invited)**B. Poumellec<sup>\*1</sup>; M. Cavillon<sup>1</sup>; J. Cao<sup>2</sup>; E. Muzi<sup>1</sup>; R. Que<sup>1</sup>; M. Lancry<sup>1</sup>

1. UPSud, SP2M, France
2. Tsinghua University, School of Materials Science and Engineering, China

**10:20 AM****(GOMD-S3-030-2022) Photochemically-Patterned Programmable Large-Area As<sub>2</sub>S<sub>3</sub> Chalcogenide Metalayers for Hybrid Refractive-Diffractive Infrared Media (Invited)**M. Kang<sup>\*1</sup>; B. Triplett<sup>2</sup>; M. Shalaginov<sup>3</sup>; S. Deckoff-Jones<sup>3</sup>; C. Blanco<sup>1</sup>; M. Truman<sup>4</sup>; T. Karnik<sup>3</sup>; D. J. McGill<sup>1</sup>; C. Popescu<sup>2</sup>; Y. Zhang<sup>1</sup>; L. Li<sup>2</sup>; S. An<sup>1</sup>; C. Fowler<sup>2</sup>; C. Schwarz<sup>2</sup>; H. Zhang<sup>1</sup>; A. Agarwal<sup>2</sup>; T. Gu<sup>2</sup>; J. Hu<sup>2</sup>; C. R. Baleine<sup>2</sup>; K. A. Richardson<sup>1</sup>

1. University of Central Florida, CREOL, College of Optics & Photonics, USA
2. Lockheed Martin Corporation, USA
3. Massachusetts Institute of Technology, USA
4. Ursinus College, USA
5. University of Massachusetts Lowell, USA

**10:50 AM****(GOMD-S3-031-2022) Structure-Terahertz Properties Relationship in Chalcogenide Glasses: Laser Irradiation**N. Tostanoski<sup>\*1</sup>; J. Musgraves<sup>2</sup>; P. Wachtel<sup>2</sup>; S. K. Sundaram<sup>1</sup>

1. Alfred University, USA
2. Rochester Precision Optics, USA

**11:10 AM****(GOMD-S3-032-2022) Formation and characterization of super-periodic rotating lattice single crystals in glass**E. J. Musterman<sup>\*1</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>1</sup>

1. Lehigh University, Materials Science and Engineering, USA
2. Lehigh University, Physics, USA

**11:30 AM****(GOMD-S3-033-2022) Crystal phase-selective laser-induced crystallization of lead bismuth gallate glass**K. J. Veenhuizen<sup>\*1</sup>; O. Magneson<sup>1</sup>; C. Barker<sup>1</sup>; A. Hearsey<sup>1</sup>; J. Marsh<sup>1</sup>; V. Dierolf<sup>1</sup>; H. Jain<sup>1</sup>

1. Lebanon Valley College, Physics, USA
2. Lehigh University, Physics, USA
3. Lehigh University, Materials Science and Engineering, USA

**11:50 AM****(GOMD-S3-034-2022) Formation of Cubic Single Crystal Architecture in Glass Via Femtosecond Laser Irradiation**C. Barker<sup>\*1</sup>; E. J. Musterman<sup>2</sup>; V. Dierolf<sup>1</sup>; H. Jain<sup>2</sup>; B. Aitken<sup>4</sup>; D. Nolan<sup>4</sup>

1. Lehigh University, Physics, USA
2. Lehigh University, Materials Science & Engineering, USA
3. Lehigh University, International Materials Institute for New Functionality in Glass, USA
4. Corning Incorporated, USA

**S4: Glass Technology and Cross-Cutting Topics****Sol-gel Processing of Glasses and Ceramic Materials**

Room: Columbia (Second floor)

Session Chair: Lisa Klein, Rutgers University

**9:20 AM****(GOMD-S4-020-2022) Real-time, Across-length-scale Characterization of Cold Sintering, a Novel Ceramic Processing Technique using Synchrotron Methods (Invited)**F. Zhang<sup>\*1</sup>; R. Maier<sup>1</sup>; I. Levin<sup>1</sup>; A. J. Allen<sup>1</sup>

1. National Institute of Standards and Technology, Materials Measurement Science Division, USA

**9:50 AM****(GOMD-S4-021-2022) Sol-Gel-Derived Core-Shell GeO<sub>2</sub>-SiO<sub>2</sub> Colloids and Their Application for 3D-Printing Optical Glass (Invited)**J. F. Destino<sup>\*1</sup>

1. Creighton University, Chemistry, USA

**10:20 AM****(GOMD-S4-022-2022) Thermal Insulation Composites Made with Ambient Drying Aerogels (Invited)**L. Lu<sup>\*1</sup>

1. Liatris Inc., R&D, USA

**10:50 AM****(GOMD-S4-023-2022) Sol-gel synthesis of a hybrid single ion conducting solid-state electrolyte with double functionalized silica backbone**G. Wang<sup>\*</sup>; V. Keshishian<sup>1</sup>; J. Kieffer<sup>1</sup>

1. University Of Michigan, USA

**11:10 AM****(GOMD-S4-024-2022) Corrosion protection of Magnesium Alloy AZ31B using melting gels obtained with different alkoxy groups**A. Samateh<sup>1</sup>; M. C. Grzenda<sup>2</sup>; J. Guzman<sup>1</sup>; J. Mosa<sup>4</sup>; L. C. Lei<sup>3</sup>; M. Aparicio<sup>4</sup>; L. C. Klein<sup>5</sup>; J. P. Singer<sup>2</sup>; A. Jitianu<sup>\*1</sup>

1. Lehman College - City University of New York, Chemistry, USA
2. Rutgers University, Department of Mechanical and Aerospace Engineering & Department of Materials Science and Engineering, USA
3. Rutgers University, Department of Mechanical and Aerospace Engineering, USA
4. Instituto de Cerámica y Vidrio, Consejo Superior de Investigaciones Científicas (CSIC), Spain
5. Rutgers University, Department of Mechanical and Aerospace Engineering, USA

**11:30 AM****(GOMD-S4-025-2022) Structural Analysis of Proton Conducting Zirconia-Phosphosilicate Hybrid Membranes**L. C. Joseph<sup>1</sup>; L. C. Klein<sup>\*1</sup>

1. Rutgers University, MS&E, USA

**S1: Fundamentals of the Glassy State****Data-based Modeling and Machine Learning for Glass Science I**

Room: Constellation C/D (Second floor)

Session Chair: Adama Tandia, Corning Incorporated

**1:20 PM****(GOMD-S1-061-2022) Modelling NMR Spectroscopy of Oxide Glasses with Machine Learning (Invited)**T. Charpentier<sup>\*</sup>; Z. CHAKER<sup>1</sup>

1. Université Paris-Saclay, CEA, CNRS, NIMBE, France

**1:50 PM****(GOMD-S1-062-2022) Finding Needles in Haystacks: Deciphering a Structural Signature of Glass Dynamics by Machine Learning (Invited)**H. Liu<sup>1</sup>; M. Bauchy<sup>\*1</sup>

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

**2:20 PM****(GOMD-S1-063-2022) Machine Learning Enables to Predict Glass Properties and Optimize Glass Composition**T. Han<sup>\*</sup>; X. Xu<sup>2</sup>; J. Huang<sup>3</sup>; A. A. Kruger<sup>4</sup>; A. Kumar<sup>1</sup>; A. Goel<sup>2</sup>

1. Missouri University of Science & Technology, Material Science and Engineering, USA
2. Rutgers University, Material Science and Engineering, USA
3. Missouri University of Science & Technology, Electrical and Computer Engineering, USA
4. U.S. Department of Energy, Office of River Protection, USA

**2:40 PM****(GOMD-S1-064-2022) Physics-informed data-driven modeling of thermoviscoelastic material behaviors**A. Vu<sup>\*</sup>; A. Siva Subramanian<sup>1</sup>; T. Grunwald<sup>1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer Institute for Production Technology IPT, Fine Machining & Optics, Germany
2. Laboratory for Machine Tools and Production Engineering (WZL) of RWTH Aachen University, Germany

**3:00 PM****(GOMD-S1-065-2022) Predicting electrical properties of Glasses as a function of composition and wavelengths**M. Zaki<sup>\*</sup>; J. Jayadeva<sup>2</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, Civil Engineering, India
2. Indian Institute of Technology Delhi, Department of Electrical Engineering, India

**3:20 PM****Break****Data-based Modeling and Machine Learning for Glass Science II**

Room: Constellation C/D (Second floor)

Session Chair: Adama Tandia, Corning Incorporated

**3:40 PM****(GOMD-S1-066-2022) Learning interaction laws in atomistic system using Lagrangian Graph Neural Networks (Invited)**R. Bhattoo<sup>\*</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, India

**4:10 PM****(GOMD-S1-067-2022) Bypassing Physics Laws to Simulate Complex Atom Dynamics by Observation-based Graph Networks (Invited)**H. Liu<sup>\*</sup>; M. Bauchy<sup>1</sup>

1. UCLA, CEE, USA

**4:40 PM****(GOMD-S1-068-2022) Low Complexity Neural Network based Accurate Prediction of Glass Properties using Physical and Chemical Descriptors**S. Bishnoi<sup>\*</sup>; R. Ravinder<sup>2</sup>; N. Krishnan<sup>2</sup>; J. Jayadeva<sup>3</sup>

1. Indian Institute of Technology Delhi, School of Interdisciplinary Research(SIRE), India
2. Indian Institute of Technology Delhi, Department of Civil Engineering, India
3. Indian Institute of Technology Delhi, Electrical Engineering, India

**5:00 PM****(GOMD-S1-069-2022) Effects of optimizer and loss function on modeling glass properties with Neural Networks**P. Ammu<sup>\*</sup>; A. Tandia<sup>1</sup>

1. Corning Incorporated, USA

**5:20 PM****(GOMD-S1-070-2022) Learning Quantum-accuracy Interatomic Potential for Silica Using Lagrangian Graph Neural Networks**R. Bhattoo<sup>\*</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, Civil Engineering Department, India

**Glass Crystallization and Glass Ceramics**

Room: Frederick (Second floor)

Session Chair: Matthew McKenzie, Corning Incorporated

**1:20 PM****(GOMD-S1-071-2022) Curved lattices of crystals formed in glass (Invited)**E. J. Musterman<sup>1</sup>; V. Dierolf<sup>1</sup>; H. Jain<sup>\*1</sup>

1. Lehigh University, International Materials Institute for New Functionality in Glass, USA

**1:50 PM****(GOMD-S1-072-2022) In-situ Measurement of Crystallization During Cooling by High Temperature Neutron Diffraction**I. Peterson<sup>\*</sup>; Y. Shi<sup>2</sup>; Y. Chen<sup>3</sup>; K. An<sup>3</sup>; J. Wright<sup>1</sup>; A. Priven<sup>4</sup>; B. Wheaton<sup>2</sup>; S. Halstead<sup>2</sup>; D. Bogdan<sup>1</sup>

1. Corning Research and Development Corporation, Process Research, USA
2. Corning Research and Development Corporation, Characterization Science and Services, USA
3. Oak Ridge National Laboratory, USA
4. Corning Research and Development Corporation, Glass Research, USA

**2:10 PM****(GOMD-S1-073-2022) Effect of electric field on glass sinter-crystallization in the Li<sub>2</sub>O-SiO<sub>2</sub> system**E. B. Ferreira<sup>\*</sup>; J. R. Murgida<sup>1</sup>; C. Magon<sup>2</sup>

1. University of São Paulo, EESC, Brazil
2. University of Sao Paulo, IFSC, Brazil

**2:30 PM****(GOMD-S1-074-2022) Electron beam heating as a new tool for fabricating novel rotating lattice single crystals in glass**E. J. Musterman\*; V. Dierolf; H. Jain<sup>1</sup>

1. Lehigh University, Materials Science and Engineering, USA
2. Lehigh University, Physics, USA

**2:50 PM****(GOMD-S1-075-2022) What particles and crystals do to the mechanical properties of glass: Case studies**T. Rouxel\*; P. Houizot<sup>1</sup>; Y. Gueguen<sup>1</sup>; J. Moriceau<sup>1</sup>; T. Lacondemine<sup>1</sup>; P. Sellappan<sup>1</sup>

1. Université de Rennes 1, Glass Mechanics, France

**3:10 PM****Break****3:30 PM****(GOMD-S1-076-2022) Nucleation – The Current State of Affairs (Invited)**

K. F. Kelton\*

1. Washington University, Physics, USA

**4:00 PM****(GOMD-S1-077-2022) Stress Dependent Phase Transition of Cristobalite Containing Glass-Ceramics**K. T. Strong\*; T. Diebold<sup>1</sup>; J. Laing<sup>2</sup>; S. Dai<sup>1</sup>; B. Lester<sup>3</sup>

1. Sandia National Laboratories, Material Mechanics and Tribology, USA
2. Sandia National Laboratories, Metallurgy and Materials Joining, USA
3. Sandia National Laboratories, Materials and Failure Modeling, USA

**4:20 PM****(GOMD-S1-078-2022) Examining the effect of the [SiO<sub>2</sub>]/[Li<sub>2</sub>O] on the microstructure and properties of lithium disilicate glass-ceramics that contain lithium tantalate as a secondary phase**A. V. DeCeanne\*; C. Ritzberger<sup>2</sup>; M. Dittmer<sup>2</sup>; M. Rampf<sup>2</sup>; J. C. Mauro<sup>1</sup>

1. Pennsylvania State University, Materials Science and Engineering, USA
2. Ivoclar Vivadent AG, Liechtenstein

**4:40 PM****(GOMD-S1-079-2022) Driving Crystallization on Silicate Melts through Metadynamics Simulations**A. Pedone\*; F. Lodesani<sup>1</sup>; S. Urata<sup>2</sup>

1. University of Modena and Reggio Emilia, Italy
2. Ashai Glass Company, Japan

**5:00 PM****(GOMD-S1-080-2022) Gillespite Glass-Ceramics**L. Moore\*; M. M. Wallen<sup>1</sup>; G. H. Beall<sup>1</sup>

1. Corning Incorporated, Glass Research, USA

**Non-oxide Glasses and Glass-ceramics II**

Room: Constellation E (Second floor)

Session Chair: Pierre Lucas, Univ of Arizona

**1:20 PM****(GOMD-S1-081-2022) Combination of theoretical and experimental data to solve the structure of telluride glasses (Invited)**D. Le Coq\*; E. Furet<sup>1</sup>; C. Boussard-Pledel<sup>1</sup>; E. Bychkov<sup>2</sup>

1. University of Rennes, ISCR, France
2. University of Littoral - Côte d'Opale, LPCA, France

**1:50 PM****(GOMD-S1-082-2022) Synthesis and Structural Investigation of Mixed Oxy-Sulfide-Nitride (MOSN) Glasses (Invited)**S. Kmiec\*; J. E. De Souza<sup>2</sup>; S. R. de Souza<sup>2</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, USA
2. UFGD - Universidade Federal da Grande Dourados, Physics, Brazil

**2:20 PM****(GOMD-S1-083-2022) Thermodynamic approach to the properties of lithium phosphorus oxynitride glasses**A. López-Grande<sup>1</sup>; F. Muñoz\*

1. Institute of Ceramics and Glass, CSIC, Spain

**2:40 PM****(GOMD-S1-084-2022) Elaboration, structure and mechanical properties of oxynitride glasses from the SiO<sub>2</sub>-BaO-Al<sub>2</sub>O<sub>3</sub>-Si<sub>3</sub>N<sub>4</sub> chemical system**A. Duval\*; B. Hehlen<sup>2</sup>; A. Moréac<sup>1</sup>; D. Massiot<sup>2</sup>; P. Houizot<sup>1</sup>; T. Rouxel<sup>1</sup>

1. Université de Rennes 1, France
2. Université Montpellier II, France
3. CEMHTI, MatRMag, France

**3:00 PM****(GOMD-S1-085-2022) Composition, properties, and SRO structures of mixed oxy-sulfide nitride glasses in the series** $\text{Na}_4\text{P}_{2-6x}\text{S}_{4.62x}\text{O}_{0.92x}; 0 \leq x \leq 0.5$ 

M. P. Martin\*

1. Iowa State University, MSE, USA

**Predicting Glass Properties**

Room: Constellation F (Second floor)

Session Chair: Alfonso Pedone, University of Modena and Reggio Emilia

**1:20 PM****(GOMD-S1-086-2022) Electronic and vibrational properties of the surface of silica and sodium silicate glasses (Invited)**Z. Zhang<sup>2</sup>; W. Kob<sup>1</sup>; S. Ispas\*

1. University of Montpellier, Lab. Charles Coulomb, France
2. Center for Alloy Innovation and Design, State Key Laboratory for Mechanical Behavior of Materials, China

**1:50 PM****(GOMD-S1-087-2022) Indentation Behaviors of Glass Studied by Classical Molecular Dynamics Simulations**H. Liu<sup>1</sup>; L. Huang\*; Y. Shi<sup>1</sup>

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

**2:10 PM****(GOMD-S1-088-2022) Prediction of Silica Glass Etching with HF Vapor Gas by Kinetic Monte Carlo Simulations**H. Park\*; A. Antony<sup>2</sup>; J. Banerjee<sup>3</sup>; G. Agnello<sup>3</sup>; N. J. Smith<sup>3</sup>

1. Corning Precision Materials, Corning Technology Center Korea, Republic of Korea
2. Corning Incorporated, Manufacturing, Technology, and Engineering Division, USA
3. Corning Incorporated, Science and Technology Division, USA

**2:30 PM****(GOMD-S1-089-2022) Transience of Mechanical Relaxation in Metallic Glass**L. Zella\*; J. Moon<sup>2</sup>; T. Egami<sup>1</sup>

1. University of Tennessee, Materials Science and Engineering, USA
2. Oak Ridge National Lab, Materials Science and Technology Division, USA

**2:50 PM****(GOMD-S1-090-2022) Theoretical estimation of dielectric loss of oxide glasses using non-equilibrium molecular dynamics simulations (Invited)**S. Urata\*; H. Hijjya<sup>1</sup>; K. Niwano<sup>1</sup>; J. Matsui<sup>2</sup>

1. AGC Inc., Japan
2. Kyushu University, Japan



**S4: Glass Technology and Cross-Cutting Topics****3D Printing of Glass**

Room: Columbia (Second floor)

Session Chair: Laurent Gallais, Institut Fresnel

**1:20 PM****(GOMD-S4-026-2022) 3D Printing of Glass Imaging Optics with High Precision using a Liquid Silica Resin (Invited)**P. Ye<sup>2</sup>; Z. Hong<sup>3</sup>; R. Liang<sup>3</sup>; D. A. Loy<sup>\*1</sup>

1. The University of Arizona, Materials Science and Engineering, USA
2. The University of Arizona, Chemistry and Biochemistry, USA
3. The University of Arizona, Wyatt College of Optical Sciences, USA

**1:50 PM****(GOMD-S4-027-2022) 3D Printed Silica with Nanoscale Resolution (Invited)**J. Lou<sup>\*1</sup>

1. Rice University, USA

**2:20 PM****(GOMD-S4-028-2022) Laser printing of fused silica parts based on multiphoton polymerization of photocurable nanosilica dispersions (Invited)**L. Gallais<sup>\*1</sup>; T. Doualle<sup>1</sup>; J. André<sup>2</sup>

1. Institut Fresnel, France
2. Laboratoire Réactions et Génie des Procédés, France

**2:50 PM****(GOMD-S4-029-2022) Optimisation of Powder Based Laser Additive Manufacturing of Soda Lime Silica Glass**F. Spirret<sup>\*1</sup>; K. Datsiou<sup>1</sup>; R. Goodridge<sup>1</sup>; I. Ashcroft<sup>1</sup>; M. Magallanes<sup>2</sup>

1. University of Nottingham, United Kingdom
2. Glass Technology Services, United Kingdom

**3:10 PM****Break****3:30 PM****(GOMD-S4-030-2022) Highly efficient, thermally robust and 3D printable green-emitting phosphor-in-glass composites**L. Qi<sup>\*1</sup>

1. Zhejiang University, China

**3:50 PM****(GOMD-S4-031-2022) Additive manufacturing of chalcogenide glasses for mid-infrared applications (Invited)**J. Troles<sup>\*1</sup>; J. Carcreff<sup>1</sup>; F. Cheviré<sup>1</sup>; R. Lebullenger<sup>1</sup>; A. Gautier<sup>1</sup>; R. Chahal<sup>2</sup>; L. Calvez<sup>1</sup>; C. Boussard-Pledel<sup>1</sup>; L. Brilland<sup>1</sup>; F. Charpentier<sup>3</sup>; H. Taniel<sup>3</sup>; Y. Guimond<sup>4</sup>; M. Rozé<sup>4</sup>; L. Szymczyk<sup>4</sup>; G. Renversez<sup>5</sup>

1. University of Rennes 1, France
2. SelenOptics, France
3. Diafir, France
4. Umicore IR Glass, France
5. Aix-Marseille Univ, Institut Fresnel, France

**Thursday, May 26, 2022****Award Lectures****Varshneya Glass Technology Lecture**

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

**8:00 AM****Introduction****8:10 AM****(GOMD-AW-005-2022) From strong bioactive glasses to tough bio-inspired glass-ceramics: A journey towards damage-resistant materials**Q. Fu<sup>\*1</sup>

1. Corning Incorporated, USA

**8:50 AM****Award Presentation****S2: Glass and Interactions with Its Environment: Fundamentals and Applications****Surfaces and Coatings**

Room: Constellation F (Second floor)

Session Chair: Matthew Linford, Stanford University

**9:20 AM****(GOMD-S2-050-2022) Non-uniform glass surface chemistry and its role in producing delaminated flakes in pharmaceutical containers (Invited)**R. Schaut<sup>\*1</sup>; S. A. Tietje<sup>1</sup>; D. Ragland<sup>1</sup>; D. Kramer<sup>2</sup>; E. Bakowska<sup>3</sup>

1. Corning Incorporated, S&T, Glass Research, USA
2. Corning Incorporated, Pharmaceutical Technologies, USA
3. Corning Incorporated, Characterization Sciences, USA

**9:50 AM****(GOMD-S2-051-2022) Modification of Multicomponent Glass Surfaces with HF Vapors**N. J. Smith<sup>\*1</sup>; G. Agnello<sup>1</sup>; J. Banerjee<sup>1</sup>; H. Park<sup>1</sup>; R. Yongsunthon<sup>1</sup>; K. Adib<sup>1</sup>; A. Antony<sup>1</sup>

1. Corning Incorporated, USA

**10:10 AM****(GOMD-S2-052-2022) Interfacial optical effects as revealed with scattering scanning near field optical microscopy (sSNOM) on acid leached soda lime silica (SLS) glass reveal limitations of plug-and-chug spectroscopy**A. L. Ogrinc<sup>\*1</sup>; Y. Zhou<sup>3</sup>; S. Hahn<sup>4</sup>; T. Gokus<sup>2</sup>; S. H. Kim<sup>1</sup>

1. Pennsylvania State University, Chemical Engineering, USA
2. neaspec, Germany
3. University of Illinois at Urbana-Champaign, USA
4. Samsung Electronics, Republic of Korea

**10:30 AM****(GOMD-S2-053-2022) Non-destructive characterization of corroded glass surfaces (Invited)**T. Kaspar<sup>\*1</sup>

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA

**11:00 AM****(GOMD-S2-054-2022) Glass surface under stress -- what do we know about the stress effect on mechanical properties?**S. H. Kim<sup>\*1</sup>; H. Liu<sup>1</sup>

1. Pennsylvania State University, Chemical Engineering & Materials Science, USA

**11:20 AM****(GOMD-S2-055-2022) Chemical and physical properties of aluminoborosilicate glass surfaces treated with alkaline solutions of variable strength and/or component ratio**G. Agnello<sup>\*1</sup>; N. J. Smith<sup>1</sup>; J. Banerjee<sup>1</sup>; M. Bell<sup>1</sup>; C. V. Cushman<sup>1</sup>; A. Antony<sup>1</sup>; H. Park<sup>1</sup>

1. Corning Incorporated, USA

**11:40 AM****(GOMD-S2-056-2022) Photothermal AFM-IR Analysis of High Extinction Coefficient Materials: A Case Study with Silica and Silicate Glasses**Y. Lin<sup>\*1</sup>; H. He<sup>2</sup>; H. Kaya<sup>3</sup>; H. Liu<sup>4</sup>; D. Ngo<sup>1</sup>; N. J. Smith<sup>4</sup>; J. Banerjee<sup>4</sup>; A. Borhan<sup>1</sup>; S. H. Kim<sup>1</sup>

1. Pennsylvania State University, Chemical Engineering, USA
2. Southwest University of Science and Technology, China
3. Pennsylvania State University, USA
4. Corning Incorporated, USA

**12:00 PM****(GOMD-S2-057-2022) Effect of Vickers Indentation Flaws on Chemical Strengthening of SLS Glass**C. Budziszewski\*; W. LaCourse<sup>1</sup>

1. Alfred University, Inamori School of Engineering, USA

**12:20 PM****(GOMD-S2-058-2022) A Tag-and-Count Approach for Quantifying Surface Silanol Densities on Fused Silica Based on Atomic Layer Deposition and High-Sensitivity Low-Energy Ion Scattering**T. Gholian Awal<sup>1</sup>; S. Prusa<sup>2</sup>; C. V. Cushman<sup>2</sup>; G. Hodges<sup>1</sup>; S. Fearn<sup>4</sup>; J. Cechal<sup>5</sup>; T. Sikola<sup>3</sup>; H. Brongersma<sup>2</sup>; M. R. Linford\*<sup>1</sup>

1. Brigham Young University, Department of Chemistry and Biochemistry, USA
2. Corning Incorporated, Science & Technology Division, USA
3. Brno University of Technology, Institute of Physical Engineering, Czechia
4. Imperial College of London, Department of Materials, United Kingdom
5. Brno University of Technology, CEITEC, Czechia
6. Eindhoven University of Technology, Department of Applied Physics, Netherlands

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Optical Fibers and Waveguides**

Room: Frederick (Second floor)

Session Chair: Jiawei Luo, OFS Laboratories

**9:20 AM****(GOMD-S3-035-2022) Engineering the characteristics of nanoparticles in preforms and optical fibers (Invited)**Z. Lu<sup>1</sup>; J. Fourmont<sup>2</sup>; I. Martin<sup>3</sup>; T. Robine<sup>1</sup>; M. Guzik<sup>4</sup>; M. Bellec<sup>1</sup>; D. Tosi<sup>5</sup>; C. Molardi<sup>2</sup>; F. Pigeonneau<sup>4</sup>; S. Chausse<sup>2</sup>; C. Guillermier<sup>2</sup>; H. Francois-Saint-Cyr<sup>6</sup>; W. Blanc\*<sup>1</sup>

1. CNRS, INPHYNI, France
2. Laboratoire de Photonique d'Angers, France
3. CAMECA Instruments Inc., USA
4. Faculty of Chemistry University of Wrocław, Poland
5. Nazarbayev University, School of Engineering and Digital Sciences, Kazakhstan
6. MINES ParisTech, PSL Research University, CEMEF, France
7. Brigham and Women's Hospital, USA
8. Thermo Fisher Scientific, USA

**9:50 AM****(GOMD-S3-036-2022) Challenges and opportunities of multi-material optical fibers (Invited)**F. Sorin\*<sup>1</sup>

1. EPFL, Switzerland

**10:20 AM****(GOMD-S3-038-2022) Elaboration and loss optimization of niobium rich borophosphate optical glass fibers**G. El Dib\*<sup>1</sup>

1. University of Limoges, Physics, France

**10:40 AM****(GOMD-S3-039-2022) Multifunctional ferromagnetic fiber robots for navigation, imaging, and optical modulation in biomedical applications**Y. Zhang\*<sup>1</sup>; J. Kim<sup>1</sup>; Y. Li<sup>1</sup>; S. Yang<sup>2</sup>; S. Hu<sup>2</sup>; H. Sontheimer<sup>3</sup>; X. Jia<sup>1</sup>

1. Virginia Tech, Department of Electrical and Computer Engineering, USA
2. Washington University in St. Louis, Biomedical engineering, USA
3. University of Virginia, Department of Neuroscience, USA

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**The American Ceramic Society**

**2022 Glass & Optical Materials Division  
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**ABSTRACT BOOK**

**May 23–26, 2022  
Baltimore, Maryland**

# Introduction

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## How to Use the Abstract Book

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Refer to the Table of Contents to determine page numbers on which specific session abstracts begin. At the beginning of each session are headings that list session title, location and session chair. Starting times for presentations and paper numbers precede each paper title. The Author Index lists each author and the page number on which their abstract can be found.

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Monday, May 23, 2022

## Award Lectures

### Stookey Lecture of Discovery

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

8:10 AM

#### (GOMD-AW-001-2022) Nanostructured Glasses (Nano-glasses): The Door to a New Glass-based Technology Age: A Glass Age

H. Gleiter\*<sup>1</sup>

1. Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology, Germany

In 1989 a new kind of non-crystalline materials – called nano-glasses – was proposed and evidenced to exist. They consist of nanometer-sized glassy regions connected by (nanometer-wide) interfacial regions with atomic and electronic structures that do not exist in melt-cooled glasses. Due to their new atomic/electronic structures, the properties of nano-glass differ from the corresponding properties of melt-cooled glasses. For example, their ductility, their biocompatibility, their catalytic and ferromagnetic properties are changed by up to several orders of magnitude. Moreover, they permit the alloying of components e.g. ionic materials (e.g. SiO) and metallic materials (e.g. PdSi glasses) that are immiscible in the crystalline state. The properties of nano-glasses may be controlled by varying the sizes and/or chemical compositions of the glassy clusters which opens the perspective of a new age of technologies - a “glass age”. A second group of nanostructured partially non-crystalline materials with tunable properties are nano-porous metals with electrolyte filled pores. By applying an external voltage between the electrolyte and the nano-porous metal their properties e.g. their superconductivity, magnetic moment, electric resistivity may be varied. Single or multi-atom switchable contacts represent a third group of these materials.

## S1: Fundamentals of the Glassy State

### Mechanical Properties of Glasses: Indentation Responses

Room: Frederick (Second floor)

Session Chair: Satoshi Yoshida, AGC Inc.

9:20 AM

#### (GOMD-S1-001-2022) Fracture and Bond Switching in Simulated Glassy Alumina and Silica

M. M. Smedskjaer\*<sup>1</sup>; T. Du<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

Alumina (Al<sub>2</sub>O<sub>3</sub>) and silica (SiO<sub>2</sub>) are important network-forming components in many oxide glasses. It is therefore important to understand how these oxides respond structurally and mechanically to applied stresses and strains. Based on molecular dynamics simulations, we here reveal to which extent the propensity of glassy Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> to exhibit nanoscale ductility is encoded in their static structures. We address this by studying the fracture response of a series of glassy Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub> systems quenched under varying pressures and cooling rates. We demonstrate that the degree of nanoductility is correlated with the number of bond switching events around Al and Si atoms, and in turn attempt to predict the tendency for bond switching based on classification-based machine learning and topological data analysis. These results are helpful for designing oxide glass formulations with improved resistance to fracture.

9:40 AM

#### (GOMD-S1-002-2022) Impact of pressure on the structure and properties of metaluminous sodium aluminoborosilicate glasses

N. Stone-Weiss\*<sup>2</sup>; B. Siboczy<sup>1</sup>; R. Sun<sup>3</sup>; N. J. Smith<sup>2</sup>; R. Youngman<sup>2</sup>; M. Bockowski<sup>4</sup>; L. Huang<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Materials Science and Engineering, USA
2. Corning Incorporated, Science and Technology Division, USA
3. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA
4. Institute of Physics Polish Academy of Sciences, Institute of High Pressure Physics, Poland

Aluminoborosilicate glasses comprise a large fraction of essential glasses used in both everyday life and for cutting edge-technological applications. These glasses show a wide range of composition-dependent properties which are exploited for applications spanning from ultra-strong cell phone cover glass and thermally resistant glasses to glasses for nuclear waste immobilization. Applying high pressure to glasses near the glass transition has been shown to significantly affect glass structure and properties, as varied pressure temperature can induce polymorphism in the glass network due to density alterations. We aim to elucidate the effects that pressure has upon structure and mechanical / elastic properties in sodium aluminoborosilicate glasses. By measuring glass structure via NMR spectroscopy and properties of samples prepared at both ambient and 1 GPa pressures, we expect to gain a complete understanding of the role that pressure plays in inducing polymorphic changes across a broad composition space and in turn how these changes impact glass performance and characteristics.

10:00 AM

#### (GOMD-S1-003-2022) Correlation of hardness of aluminosilicates and glass network connectivity and atomic packing density

H. Lee\*<sup>1</sup>; W. M. Carty<sup>1</sup>

1. Alfred University, New York State college of ceramics at Alfred University, USA

The hardness of alkaline earth aluminosilicate glasses was evaluated focusing on the glass network connectivity and the atomic packing density of systems. Vickers hardness of the glasses were evaluated in two steps: the calcium aluminosilicate system and then a range of RO modifiers, including RO blends. The hardness results for CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> (CAS) glasses demonstrated that hardness is strongly correlated with the alumina level and with the melting behavior as predicted by the phase diagram. The hardness of CAS and MgO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> (MAS) glasses were similar, ranging from 6.7 GPa to 7.2 GPa, but the replacement of CaO with MgO produced only a marginal increase in hardness. Conversely, the blending of CaO with SrO and BaO generally resulted in a decrease in hardness. The sensitivity to alumina, however, was much greater ranging from ~4.5 to a maximum of ~8.2 GPa. Overall, it was concluded that, in general, the hardness of aluminosilicate glasses correlates to melting behavior, and that within specific compositions, with the composite cation field strength (CFS) of the modifier cations.

10:20 AM

#### (GOMD-S1-004-2022) Impact of modifier field strength on hardness, crack resistance, and charge distribution in single modifier aluminoborosilicate glasses

A. L. Fry\*<sup>4</sup>; I. Slagle<sup>2</sup>; H. Hawbaker<sup>2</sup>; C. George<sup>3</sup>; S. Feller<sup>2</sup>; S. H. Kim<sup>1</sup>; J. C. Mauro<sup>4</sup>

1. Pennsylvania State University, Chemical Engineering, USA
2. Coe College, Physics, USA
3. Pennsylvania State University, Chemistry, USA
4. Pennsylvania State University, Materials Science and Engineering, USA

The interaction among glass formers and modifiers (NWMs) are generally understood in oxide glasses, but how the species of modifier impacts the mechanical performance of aluminoborosilicate glasses is not well studied. This work explores the indentation

behaviors of six, single modifier aluminoborosilicate (ABS) glasses with respect to modifier field strength (FS). Three alkali and three alkaline earth ABS glasses were designed with ~10mol.% NWM and [NWM]  $\approx$  [Al<sub>2</sub>O<sub>3</sub>], to test modifier FS impact at low concentrations and to maximize three-coordinated boron. It has been found that both hardness and crack resistance increase with increasing FS in these ABS systems, a concept historically contradictory. Using <sup>11</sup>B, <sup>27</sup>Al, and <sup>29</sup>Si solid state NMR, this work provides evidence of how charge distributions differ as a function of NWM species, and how this relates to the observed indentation behaviors.

**10:40 AM**

### **(GOMD-S1-005-2022) Hard and crack-resistant glass**

A. Yadav<sup>\*1</sup>; A. Goel<sup>1</sup>

1. Rutgers, The State University of New Jersey, Materials Science & Engineering, USA

Realization of hard and crack-resistant bulk oxide glasses by melt-quenching is always remained desirable in the arena of glass science and glass technology, as it would pave the way towards new glass applications and reduce the overall manufacturing cost. The mechanical properties of the glasses are controlled by their atomic-scale structure, which in turn depends on the chemical composition. Therefore, a careful compositional designing of glass seems an appealing approach to further improve the intrinsic strength and damage resistance of glasses. Following this methodology, we are reporting here the invention of a novel melt-quenched (melting temperature  $\leq 1650^\circ\text{C}$ ) aluminoborosilicate glass possessing both high hardness ( $H_v \geq 7.5$  GPa) as well as crack-resistance ( $CR \geq 26.5$  N) ever reported. This glass also possesses the transmittance  $\geq 88\%$ , Young's modulus  $\sim 112$  GPa, and Poisson's ratio  $\sim 0.28$ . The <sup>27</sup>Al & <sup>11</sup>B NMR analysis of the glass shows that the majority of Al is in 4-fold ( $\sim 46\%$ ) & 5-fold ( $\sim 43\%$ ) coordination & 90% of the B is in 3-fold coordination. The indentation-driven changes in localized structure are also studied using Raman spectroscopy to understand how the applied mechanical energy during indentation is consumed.

**11:00 AM**

### **(GOMD-S1-006-2022) Lateral-pushing induced surface lift-up during nanoindentation of silicate glass**

L. Ding<sup>\*1</sup>; Q. Zheng<sup>2</sup>; J. C. Mauro<sup>3</sup>

1. Donghua University, College of Materials Science and Engineering, China
2. Qilu University of Technology, School of Materials Science and Engineering, China
3. The Pennsylvania State University, Department of Materials Science and Engineering, USA

Shear flow and/or densification have been long considered as the main mechanisms accounting for inelastic deformation during indentation of silicate glasses. However, the role of inelastic deformation during indentation of silicate glass is still debated. In this work, the cube-corner indenter was chosen to perform the nanoindentation tests on four different types of silicate glasses with a penetration depth of up to 0.5  $\mu\text{m}$ . A 3D surface analysis method is developed to quantify the amplitude of the impression field. Based on this newly developed analysis approach, we have found that the shear flow and densification induced inelastic deformation of silicate glasses are visible as indentation, as pile-up close to the indent, and as lift-up far away from the indent. The lift-up mechanism is revealed for the first time, which complements the previous well-accepted pile-up description. The lift-up region is due to the increasing width of the indenter as it is pushed into the glass, which corresponds to the amount of glass volume pushed away laterally (lateral-pushing) and can contribute up to  $\sim 25\%$  of the total volume above the original surface in soda-lime silicate glass. We believe this better quantification of inelastic deformation will contribute to revealing the structural evolution during nanoindentation of silicate glass.

**11:20 AM**

### **(GOMD-S1-007-2022) 3D Raman Mapping of Glass Indentation Stress Fields**

A. J. Bellafatto<sup>\*1</sup>; I. Reimanis<sup>1</sup>

1. Colorado School of Mines, Materials Science, USA

Crack initiation associated with contact damage is of great interest for glass that experiences mechanical loads. The stress field under an indent is dependent on a variety of factors, including the glass type, indenter acuity, amount and type of plasticity, and the presence of cracks. In the present work, Raman mapping is used to describe the stress state in silica and soda lime silicate after indentation. Details of the measurement, including stress calibration and spatial resolution are described.

**11:40 AM**

### **(GOMD-S1-008-2022) Crack nucleation and propagation mechanisms in amorphous silica**

Z. Hossain<sup>\*1</sup>

1. University of Delaware, Mechanical Engineering, USA

Applying a combination of atomistic simulations and continuum scale analysis, we report the fundamental mechanisms that govern fracture in amorphous silica. Our results suggest that crack nucleation and propagation are governed by chainlike nanoscale stress-fibers. They belong to a set of interacting tetrahedral structures, and they form and break continuously during the crack nucleation and propagation process. They are responsible for localizing stress at the crack nucleation site or propagating crack front. As soon as the stress-fibers reach a critical density the material starts nucleating cracks or leads to propagation of the initial crack. The density of the stress-fibers intensifies at the crack-tip with increased deformation at the remote boundary. Consequently, the crack-tip stress fields vary as  $1/r$ , as opposed to continuum scale approximation of square-root singularity. Furthermore, the presence of nanometer-scale holes or pores within the interaction distance of a crack-tip intensifies the stress state of the stress-fibers near the crack front. The results unambiguously demonstrate strong heterogeneous character of the amorphous material and the distinctive roles of the individual species that make it behave very differently from what is seen in homogeneous and crystalline materials from continuum scale theories.

## **S2: Glass and Interactions with Its Environment: Fundamentals and Applications**

### **Dissolution and Interfacial Reactions I: Dissolution behavior as a Function of Glass Composition**

Room: Constellation C/D (Second floor)

Session Chairs: Alfonso Pedone, University of Modena and Reggio Emilia; Stéphane Gin, CEA

**9:20 AM**

### **(GOMD-S2-001-2022) The Composition Dependence of Glass Dissolution Rate (Invited)**

N. J. Smith<sup>\*1</sup>; R. Schaut<sup>1</sup>; E. Bakowska<sup>1</sup>; J. P. Icenhower<sup>1</sup>; A. Tandia<sup>1</sup>; S. Goyal<sup>1</sup>; R. Youngman<sup>1</sup>

1. Corning Incorporated, USA

Predicting the composition dependence of glass chemical durability has been a long-standing challenge in the field of glass science, as well as with the development of new multicomponent glasses for applications as diverse as displays, cover glasses, wafer substrates, and advanced optics. At Corning, we have set about a multi-year experimental and modeling effort to tackle this problem, largely

aimed at understanding the critical principles underlying forward rate behavior from the standpoint of glass structure, and with timeframes and chemistries that impact technical glass products. In this talk, I will recap some of the key learnings from this endeavor, describing experiments with over 50 simplified glass compositions, the translation of composition to important aspects of structure in the glass network, and finally its manifestation in dissolution rates over a variety of dilute aqueous solutions from strong acids to strong bases. These data and insights have led to new models of glass corrosion that can be used to predict practical durability behavior important to commercial glass products.

9:50 AM

**(GOMD-S2-002-2022) Deciphering the non-linear impact of Al on chemical durability of silicate glass**

K. Damodaran<sup>\*1</sup>; J. Delaye<sup>1</sup>; A. Kalinichev<sup>1</sup>; S. Gin<sup>1</sup>

1. CEA, France

Role of Al in aluminosilicate glasses remains misunderstood; at low concentration it increases the glass resistance to hydrolysis whereas at high concentration an opposite effect is observed. To understand the origin of the phenomenon at atomic level, we performed 577 MD simulations through potential mean force (PMF) method to estimate the activation barriers and to correlate statistically with their corresponding structural features of silicate and aluminosilicate glasses. PMF simulation results validated by the experimental studies revealed that Al is very easy to dissociate, but increases the resistance of glass towards water through significantly increasing both the strength of Si and network connectivity. In contrast, at high Al concentration, preferential dissolution of Al weakens the silicate network, and so the glass resistance becomes very poor. Activation barrier for dissociating bonds around Al is 0.46eV, which is significantly less than Si in pure silicate (1.22eV) and Si in aluminosilicate glass (1.34eV). Si with Al as second neighbour had significantly higher activation energy than Si in pure silicate glass.

10:10 AM

**(GOMD-S2-003-2022) Glass Formation and Chemical Durability in Copper Borates**

C. Calahoo<sup>\*1</sup>; P. N. DeMaere<sup>1</sup>; S. Adab<sup>2</sup>; Y. Boluk<sup>1</sup>; W. Wall<sup>2</sup>

1. University of Alberta, Civil Engineering, Canada

2. Genics Inc., Canada

Typically, borate is only a secondary additive to a primary glass former, however copper borates are used in the wood industry where the dissolution products prevent mold, decay, and termites, doubling or trebling the lifetime of wood products. To further this application, we characterize the binary copper-borate and ternary sodium-copper-borate glass systems. We investigate the glass-forming region of these glass systems and report the macroscopic properties, such as density, elastic moduli and  $T_g$ . Furthermore, we aim to understand the chemical durability in different conditions such as pH and temperature as well as static vs. continuous dissolution as a function of composition. We use ICP-MS to measure concentration profiles to gain insight on the dissolution mechanism, i.e., incongruous vs. congruous. Additionally, the effect of  $\text{Cu}^{2+}$  vs.  $\text{Cu}^+$  is correlated to trends in the macroscopic properties. Finally, the glass structure, as elucidated by Raman, IR and NMR spectroscopy, is related to the macroscopic properties as well.

10:30 AM

**(GOMD-S2-004-2022) Structure of Calcium Aluminosilicate Glasses and its Role in Governing Dissolution Kinetics**

J. P. Icenhower<sup>\*1</sup>; N. J. Smith<sup>2</sup>; R. Youngman<sup>2</sup>; D. K. Shuh<sup>3</sup>; H. McMahon<sup>1</sup>; M. Riesbeck<sup>1</sup>

1. Corning Incorporated, Chemical Analysis, USA

2. Corning Incorporated, USA

3. Lawrence Berkeley National Laboratory, USA

Calcium aluminosilicate glasses represent baseline chemical compositions for many commercially important glasses, yet the dissolution kinetics of such materials have not been adequately ascertained. We determined the dissolution rates of eleven glasses, which spanned three series of compositions from metaluminous, peralkaline, and peraluminous, by running powdered samples in a single-pass flow-through (SPFT) system at pH 7.5 and 75 °C. Moieties of Al were also characterized by MAS-NMR on all eleven samples while the Si K-edge was documented for four glasses using XANES at the Canadian and Advanced Light Sources (CLS and ALS). These data enabled us to contemplate links between glass structure and dissolution kinetics. For the metaluminous glasses, rates decreased moderately with increasing silica concentrations, with no strong correlation observed with Al species, such as  $^{27}\text{Al}$ . Rates of dissolution for peralkaline glasses also decreased with increasing Si, but less sharply. Again, dissolution of peralkaline glasses did not strongly correlate with  $^{27}\text{Al}$ . The data are consistent with dissolution rates as a function of Si content of glass, with more minor correlations with molar Si/Al ratios.

10:50 AM

**(GOMD-S2-005-2022) Dissolution behavior and kinetics of alkali/alkaline-earth aluminoborosilicate glasses in acidic media: Impact of high ionic field strength non-framework cations**

Q. Qin<sup>\*1</sup>; N. Stone-Weiss<sup>1</sup>; T. Zhao<sup>3</sup>; P. Mukherjee<sup>2</sup>; J. Ren<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science and Engineering, USA

2. Michigan Technological University, Materials Science and Engineering, USA

3. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Key Laboratory of Materials for High-Power Laser, China

Selective chemical etching in acidic medium has shown promising applications in developing thinner, higher performance display glasses and glass substrates, as it can tune the properties of very thin glass material without significantly altering its thickness. However, such technique must be performed in a highly controlled and well-predicted manner to achieve targeted properties, and therefore requires a comprehensive understanding of the fundamental science governing the glass-acid interactions — particularly relating to the impact of common constituent oxides. The majority of functional glasses contain non-framework high field-strength cations (HFSCs), for example,  $\text{Ca}^{2+}$ ,  $\text{Ti}^{4+}$  and  $\text{Zr}^{4+}$ . However, their impact on the acidic corrosion of aluminoborosilicate glasses remained undeciphered. Accordingly, in this work we have synthesized a series of alkali/alkaline-earth aluminoborosilicate glasses containing different non-framework high field strength cations (i.e.,  $\text{La}^{3+}$ ,  $\text{Ti}^{4+}$ ,  $\text{Zr}^{4+}$ ,  $\text{Nb}^{5+}$ ) and investigate their dissolution behavior in Tris-HCl solution (pH=2). Employing a suite of state-of-the-art spectroscopic techniques, we demonstrate the impact of these HFSCs on the reaction kinetics and structural evolution of the glasses during the acidic dissolution.

11:10 AM

**(GOMD-S2-006-2022) Dissolution Reaction Products from  $\text{Na}_2\text{O-CaO-B}_2\text{O}_3\text{-P}_2\text{O}_5$  Glasses in Simulated Body Fluids**

R. L. Blatt<sup>\*1</sup>; R. Brow<sup>1</sup>

1. Missouri University of Science & Technology, Materials Science and Engineering, USA

Glass powders with the nominal compositions (mol%)  $(100-y)(0.5\text{Na}_2\text{O}-0.5\text{CaO})-x\text{B}_2\text{O}_3-(y-x)\text{P}_2\text{O}_5$  ( $40 \leq y \leq 70$  and  $0 \leq x \leq y$ ) were reacted in simulated body fluid (SBF) at 37°C for up to 168 hours.



Across all series, dissolution rates initially decreased with the addition of  $B_2O_3$ , but subsequently increased with further additions, and these rates can be related to the evolution of the glass-forming network. The pH of the SBF solution increased from 2 to 8 with increasing  $B_2O_3$  contents, reflecting the relative strengths of the phosphoric and boric acids released on dissolution. Calcium-phosphate (CP) colloidal particles were released to the SBF solution and CP phases precipitated on the surfaces of the borate-rich glasses. The nature of these phases changed with glass composition and were dependent both on the local pH and on the types of anions released from the dissolving glasses.

### 11:30 AM

#### (GOMD-S2-007-2022) Stirred Reactor Coupon Analysis – A Round Robin Study

J. V. Ryan<sup>\*1</sup>; B. Parruzot<sup>2</sup>; J. Reiser<sup>2</sup>; S. Cooley<sup>2</sup>; D. Swanberg<sup>3</sup>; G. L. Smith<sup>2</sup>

1. Pacific Northwest National Lab, Advanced Processing and Applications, USA
2. Pacific Northwest National Lab, Energy and Environment, USA
3. Washington River Protection Systems, USA

At the U.S. Department of Energy Hanford Site, modelling of the long-term dissolution of borosilicate glass waste forms for immobilized low activity waste (ILAW) is done in part using an equation based on transition state theory (TST). The rate model is parameterized partially by measuring the steady-state dissolution rate of glass in dilute conditions over a range of temperatures and pH values. Previously tested using the Single-Pass Flow Through method, a higher throughput test was designed to corrode monolithic glass samples in a large, stirred reactor. The dissolution rate is determined by the change in height at the end of the test between a protected area of glass monolith samples and the receded corroded surface. The newly christened Stirred Reactor Coupon Analysis (SRCA) was successfully used to parameterize an expanded glass composition range designed to immobilize low activity nuclear waste at the Hanford site. With the goal of standardizing the SRCA test, a round robin study was initiated to examine differences in results among the 12 collaborating laboratories. In this presentation, selected round-robin data will be shown to demonstrate the repeatability and precision of the SRCA test.

### Glasses and Glass-ceramics for Healthcare

Room: Columbia (Second floor)

Session Chair: Hrishikesh Kamat, Glidewell Dental

### 9:20 AM

#### (GOMD-S2-008-2022) Multifunctional bioactive glasses doped with therapeutic ions/nanoparticles (Invited)

M. Miola<sup>1</sup>; E. Verné<sup>\*1</sup>

1. Politecnico di Torino, DISAT, Italy

Bioactive glasses have been widely investigated for their ability to release ions with therapeutic effect and it has been demonstrated that the controlled release of specific ions can stimulate several processes that regulate the regeneration of hard and soft tissues. In this work we present a review of recent studies driven by the authors in the design of innovative multifunctional glasses compositions to induce specific biological responses in hard and soft tissue regeneration. Various bioactive glasses (synthesized by sol-gel or melt and quenching process) doped with therapeutic ions or metallic nanoparticles (such as Mn, Sr, B, Mg, Zn, Cu, Te) have been designed in different forms (bulk, powders, scaffolds, composites and coatings) and investigated for their morphological, compositional, structural properties as well as in vitro reactivity and biological response. Depending on the glass composition and the doping element, synergistic and multifunctional activities have been assessed in different experimental model, ranging from osteoinductive, antibacterial and anti-inflammatory properties up to

proangiogenic and antitumor ones. Our results confirm that doping of bioactive glasses with therapeutic ions/nanoparticles has potential for promoting healing of both hard and soft tissues.

### 9:50 AM

#### (GOMD-S2-009-2022) Glass-Ceramic Scintillators for Indirect Digital Radiography

E. Moore<sup>\*1</sup>; R. L. Leonard<sup>1</sup>; J. A. Johnson<sup>1</sup>; A. M. Thomas<sup>1</sup>; A. R. Lubinsky<sup>2</sup>; A. Howansky<sup>2</sup>

1. University of Tennessee Space Institute, MABE, USA
2. Stony Brook University, USA

Indirect flat panel detectors (I-FPDs) employ a scintillator to convert x-rays into visible light, which is then utilized to create a digital radiograph. The I-FPDs used today have poor quantum efficiencies at high x-ray energies due to unabsorbed x-rays, which pass through the I-FPDs undetected. By incorporating a glass-ceramic scintillator as an additional x-ray conversion screen into a bidirectional I-FPD more x-rays would be detected, leading to better detective quantum efficiencies. This study evaluates the use of oxyhalide glass ceramics, doped with rare earths, for use as an additional x-ray conversion screen. The ability to precipitate  $CaF_2$  or other crystals in a controlled way in these glasses to prevent light trapping is explored. Several series of glass samples doped with europium or terbium were synthesized, varying the amount of crystalline precursor. The samples were then heat treated to precipitate crystallites, whose presence was confirmed using x-ray diffraction and phosphorimetry. The detected light output for the samples was compared against a commercial conversion screen. The x-ray emission spectra confirmed that the light output was primarily from the rare earth dopant and matches well with the quantum efficiency curve of silicon photodiodes. These results show that  $CaF_2$  crystals can be precipitated in a controlled manner in these glasses, reducing the amount of light trapping in the samples.

### 10:10 AM

#### (GOMD-S2-010-2022) Human Adipose Stem Cells Viability on Ag-doped Bioactive Glass Obtained by Ion Exchange

M. S. Lallukka<sup>\*1</sup>; A. Houaoui<sup>2</sup>; M. Miola<sup>1</sup>; J. Massera<sup>2</sup>; E. Verné<sup>1</sup>

1. Politecnico di Torino, Department of Applied Science and Technology, Italy
2. Tampere University, Faculty of Medicine and Health Technology, Finland

Bioactive glasses doped with antibacterial ions represent a viable option to provide a bioactive environment and simultaneously prevent biofilm formation during bone augmentation surgery. However, added challenge is their cytocompatibility, which could be compromised due to possible dopant toxicity. In this work, a melt-derived bioactive glass doped with Ag (Ag-SBA2) via ion exchange is evaluated regarding its cytocompatibility. The viability and proliferation of human adipose stem cells (hASCs) were studied upon direct culture on glass discs, with and without pre-incubation, and in medium containing glass dissolution products. The effect of fibronectin adsorption on samples was also studied in direct culture. Ag-SBA2 was found to elicit initial inhibitory effect on cell viability. However, cells remain viable when cultured directly on pre-treated discs, or with the glass dissolution products. This suggests that the cytotoxicity seems to arise from the contact toxicity of the glass surface. The cytocompatibility can be improved by fibronectin adsorption, which is seen as increased cell viability and proliferation. Our findings suggest that Ag-SBA2 has potential for treating early infection, without compromising long term bioactivity. This work has received funding from the European Union and it participates in a Marie Curie Action (“H2020-MSCA-ITN-2019 – PREMURSA – GA n° 860462”)



10:30 AM

**(GOMD-S2-011-2022) Bioactive sol-gel borate glasses for regenerative engineering (Invited)**W. C. Lepry<sup>1</sup>; S. Naseri<sup>1</sup>; E. Rezabeigi<sup>1</sup>; S. N. Nazhat<sup>\*1</sup>

1. McGill University, Mining and Materials Engineering, Canada

Sol-gel also offers numerous advantages over the melt-quench processing of bioactive glasses, such as increased compositional and textural variation, as well as reduced processing temperatures, which impact glass dissolution rates and potentially widens their applications to beyond mineralized tissue repair. This presentation will give an overview of our recent advances in the sol-gel processing of highly bioactive borate-based glasses (SGBGs). We have demonstrated that a wide compositional range of SGBGs, with at least two-orders of magnitude greater specific surface areas and pore volumes compared to their melt-quench equivalents, can be processed through sol-gel. These gains in textural properties result in higher glass dissolution and ionic release rates and at least a 25-fold increase in carbonated hydroxyapatite (CHA) conversion rate, *in vitro*. Through SGBG functionalization, these CHA conversion rates have also been realized in rapidly mineralizing injectable and printable osteoid-like dense fibrillar collagen hydrogels, both *in vitro* and *in vivo*. More recently, we have demonstrated the borate anomaly over a wide compositional range in a sol-gel derived binary alkaline-earth, CaO-B<sub>2</sub>O<sub>3</sub> system, in terms of both structural and textural properties, which we believe will provide the basis for tailoring SGBGs to target mineralized tissue regeneration, as well as antibacterial and wound healing applications.

11:00 AM

**(GOMD-S2-012-2022) Tribo-corrosion Studies of 45S5 Bioglass in Aqueous Media**S. R. Keshri<sup>\*1</sup>; S. Sahoo<sup>1</sup>; K. S<sup>1</sup>; N. Krishnan<sup>2</sup>; N. N. Gosvami<sup>1</sup>

1. Indian Institute of Technology Delhi, Materials Science & Engineering, India
2. Indian Institute of Technology Delhi, Civil Engineering, India

Metal implants used for diseased and deformed bones and teeth may cause stress shielding, cytotoxicity and genotoxicity. Additionally, autografts may also lead to donor site morbidity. Hence, tissue regeneration using Bioactive glasses can be considered as the best option for the treatment of diseased and deformed bones and teeth. The present work studies the tribo-corrosion behavior of 45S5 Bioglass in the presence of aqueous media such as DI water and simulated body fluid (SBF) to simulate the exact physiological conditions, the bioglass will be subjected to inside a human body. It will further help to understand the various wear mechanisms and wear rate occurring in the presence of bio-mechano-chemical environment and the surface stability of the bioglass, facilitating to synthesize a bioglass with tailored bioactivity and mechanical properties. The wear mechanisms will be evaluated using Scanning Electron Microscopy, and the wear volume and rate will be calculated using profilometry results. A change in the coefficient of friction will help us to evaluate the formation of tribolayer if any and its function in determining the mechanical property of the bioglass. FTIR and Raman spectroscopy will help in determining the formation of any complexes in the glass surface after being subjected to tribo-corrosion.

11:20 AM

**(GOMD-S2-013-2022) Sol-gel synthesis of spherical bioactive glass particles containing boron and copper**E. Piatti<sup>\*1</sup>; M. Miola<sup>1</sup>; E. Verne<sup>1</sup>

1. Politecnico di Torino, Department of Applied Science and Technology, Italy

Bioactive glasses (BGs) can bond to living tissues, forming a hydroxyapatite interface layer and stimulating new tissue growth. The sol-gel synthesis allows to synthesize BGs with many compositions and shapes, but the synthesis of monodisperse spherical nanoparticles (NPs) containing metallic doping ions is still

challenging. The aim of this work was to optimize our previous synthesis of innovative sol-gel B- and Cu-doped BG NPs, carefully evaluating many parameters, like initial pH condition, mixing method, amount and concentration of ammonia solution, addition timing of Ca precursor, use of centrifugation, freezing and lyophilization. B- and Cu-doped spherical BG particles were produced 1) mixing a solution containing the Si precursor with a solution containing the catalyst 2) centrifuging 3) adding the other precursors 4) centrifuging 6) drying 7) calcinating. SEM-EDS, DLS, BET, FTIR, XRD, and acellular bioactivity test were performed. This synthesis allowed to obtain particles with a good ion incorporation, a spherical shape and a satisfying dispersion. These particles were also highly bioactive (since the first day of the bioactivity test). To conclude, we successfully optimize our synthesis, enhancing particle shape, dispersion and bioactivity. In addition, the incorporation of antibacterial and angiogenic ions (like B and Cu) makes our BGs promising for both hard and soft tissue engineering.

11:40 AM

**(GOMD-S2-014-2022) Synthesizing Nanoceria with Varied Ratios of Ce<sup>3+</sup>/Ce<sup>4+</sup> Using Soluble Borate Glass**K. S. Ranasinghe<sup>\*1</sup>; R. Singh<sup>2</sup>; A. Vasquez<sup>2</sup>

1. Kennesaw State University, Physics, USA
2. Kennesaw State University, Chemistry and Biochemistry, USA

Controlling the formation of Ce<sub>2</sub>O<sub>3</sub> and CeO<sub>2</sub> nanoparticles are especially challenging via common methods that have been used to synthesize nanoceria due to the unstable nature of Ce<sub>2</sub>O<sub>3</sub>. A soluble bioactive borate glass was used to create these two types of nanoparticles with identified ratios of Ce<sup>3+</sup>/Ce<sup>4+</sup> by controlling the melting parameters. X-ray Near-Edge Structure (XANES) spectroscopy was used to calculate the Ce<sup>3+</sup>/Ce<sup>4+</sup>. Results show that these nanoceria are hermetically sealed within the glass with specific ratios and released when the glass dissolves in water with Ce<sup>3+</sup>/Ce<sup>4+</sup> ratios intact. Further, these extracted nanoceria of 2-5nm in size consist of several different structures. The extracted nanoceria exhibited multivalency and the three phases, Ce<sub>2</sub>O<sub>3</sub>, Ce<sub>7</sub>O<sub>12</sub>, and Ce<sub>11</sub>O<sub>20</sub>, contributed to the Ce<sup>3+</sup> content within the nanoceria. Further, we have observed a CeO<sub>1.66</sub> phase which has been identified as a quasi-stable state in the extracted nanoceria, and calculated the lattice expansion in these nanocrystals.

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Optical and Photonic Glasses and Glass-ceramics I**

Room: Constellation E (Second floor)

Session Chair: Lee Casalena

9:20 AM

**(GOMD-S3-001-2022) Glass-ceramics or composites for infrared luminescence properties (Invited)**V. Jubera<sup>\*1</sup>

1. Université de Bordeaux, ICMCB, France

To increase functionality of optical materials requires the combination of several properties. Glass ceramics or composites materials provides both the shaping facilities and the efficiency of the crystalline phase. It is therefore important today to work around innovative compositions whose sensitivity under external stimuli or laser irradiation makes it possible to generate new linear or non-linear optical properties. The increase in functionality has to be based on the synthesis of new materials. In the case of glass ceramics or composites, the control of local changes in composition, mechanical stresses, reactivity to interfaces or density is thus crucial. It is essential to master the compositions-structure-properties correlations within these complex systems while controlling the synthesis.

9:50 AM

**(GOMD-S3-002-2022) Luminescent properties of nanostructured glass-ceramic thin films and their potential for UV-pumped white light LED applications**

R. L. Leonard<sup>\*1</sup>; C. W. Bond<sup>1</sup>; Y. Jin<sup>4</sup>; P. Gómez-Rodríguez<sup>3</sup>; E. Nieto<sup>3</sup>; J. Gonzalo<sup>3</sup>; R. Serna<sup>3</sup>; A. Petford-Long<sup>2</sup>; J. A. Johnson<sup>1</sup>

1. University of Tennessee Space Institute, Mechanical, Aerospace, and Biomedical Engineering, USA
2. Argonne National Laboratory, Materials Science Division, USA
3. Instituto de Optica CSIC, Laser Processing Group, Spain
4. Northwestern University, Materials Science and Engineering, USA

Light emitting diodes (LEDs) are ubiquitous in the modern world. Commercially-available white light LEDs often employ two or more phosphors to create broadband emission. Ultraviolet (UV)-pumped white light LEDs, which downshift a portion of the UV photon to produce broadband visible emission, may lead to a simplified manufacturing process. The authors hypothesize that the manipulation of structure in a nanolayered luminescent material will allow control over emission properties. A series of structured thin films consisting of aluminum oxide, barium fluoride, and europium oxide nanolayers were synthesized by pulsed laser deposition. Subsequent heat treatments were used to alter the composition of the individual layers. The emission spectra were measured for the samples in both the as-made state and after heat treatment. The ability to change the nanolayer structure to affect luminescent properties was demonstrated by altering the coordinate environment of europium. For the samples, chromaticity coordinates ranged from  $x = 0.26-0.29$  and  $y = 0.32-0.35$ , which demonstrates a potential application in UV-pumped white light LEDs.

10:10 AM

**(GOMD-S3-003-2022) Photoluminescence Enhancement in Eu/CdS co-doped chloroborosilicate glass-ceramics by heat treatment**

N. Shasmal<sup>\*1</sup>; W. G. Faria<sup>2</sup>; A. S. de Camargo<sup>2</sup>; A. Rodrigues<sup>1</sup>

1. Federal University of Sao Carlos, LaMaV, Brazil
2. University of São Paulo, São Carlos Institute of Physics, LEMAF – Laboratório de Espectroscopia de Materiais Funcionais, Brazil

The effect of heat treatment was studied on Eu/CdS co-doped chloroborosilicate glass having composition  $37.8\text{SiO}_2-27\text{B}_2\text{O}_3-18\text{BaO}-3.6\text{K}_2\text{O}-3.6\text{Al}_2\text{O}_3-10\text{BaCl}_2$  (mol%). The glasses were heat treated at  $650^\circ\text{C}$  for several lengths of time. Transmission electron microscopy revealed the presence of CdS quantum dots (QDs) in the heat-treated glasses. X-ray diffraction study confirmed the formation of glass-ceramics, with the presence of  $\text{BaCl}_2$ -based phases. When heat-treated, all the Eu/CdS co-doped glasses showed an intense enhancement in  $\text{Eu}^{3+}/\text{Eu}^{2+}$  emissions up to 30 or 40 hours, followed by a gradual decrease. The initial increase is due to the formation of low-phonon energy  $\text{BaCl}_2$ -based crystalline phases as well as the generation and growth of CdS QDs. The subsequent decrease in PL intensity is due to the concentration quenching effect of the QDs. The rate of enhancement was significantly higher when glasses formed opaque glass-ceramics due to the glass crystallization which creates an environment of the Eu ions with low phonon energy, thus reducing the non-radiative loss. A scattering effect provoked by the presence of crystals also contributes to the increase in PL intensity. The maximum enhancement due to the CdS co-doping and glass crystallization was observed to be 400 times as compared to the non heat-treated glass containing the same amount of Eu.

10:30 AM

**(GOMD-S3-004-2022) Novel oxide glasses via non-traditional processing**

A. Floyd<sup>\*5</sup>; V. Nguyen<sup>1</sup>; R. Bekele<sup>6</sup>; J. Myers<sup>3</sup>; D. Gibson<sup>3</sup>; S. Bayya<sup>3</sup>; W. Kim<sup>1</sup>; J. Frantz<sup>4</sup>; D. Rhonehouse<sup>3</sup>; J. Sanghera<sup>2</sup>

1. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5621, USA
2. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5620, USA
3. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5622, USA
4. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5624, USA
5. Jacobs, On-site contractor for NRL Code 5622, USA
6. University Research Foundation, On-site contractor for NRL Code 5624, USA

Novel oxide glasses have been demonstrated through the use of non-traditional processing techniques. The non-traditional oxide glasses created using these processes have demonstrated exceptional properties due to the diverse and unique structures that can be formed. In addition, the kinetics of these processes have allowed formation of glasses with high concentrations of rare earth oxide that can act as a host to enable laser materials. We will discuss our recent efforts in developing novel passive and active glasses for use in IR laser applications and Vis/IR Gradient Index (GRIN) optics. Information on optical, physical, thermal, thermodynamic and mechanical properties as well as laser performance data will be presented.

10:50 AM

**(GOMD-S3-005-2022) Structure analysis of  $\text{CaO-WO}_3\text{-B}_2\text{O}_3$  glass and thermal evolution to Glass-Ceramics bearing Calcium Tungstate crystals with enhancement photoluminescence by  $\text{Eu}^{3+}$  doping**

T. Otsuka<sup>\*1</sup>; M. Brehl<sup>2</sup>; M. Cicconi<sup>2</sup>; D. de Ligny<sup>2</sup>; T. Hayakawa<sup>1</sup>

1. Nagoya Institute of Technology, Life Science and Applied Chemistry, Japan
2. University of Erlangen-Nuremberg, Department of Materials Science and Engineering, Germany

Thermal evolutions of calcium-tungstate-borate glasses were investigated for the development of luminescent glass-ceramics by using  $\text{Eu}^{3+}$  dopant in a borate glass matrix with calcium tungstate, which was expected to have a combined character of glass and ceramics. XRD patterns showed that single-phase precipitation of  $\text{CaWO}_4$  crystals in borate glass matrix was possible by heat-treatment at a temperature higher than glass transition temperature  $T_g$  for  $(100-x)(33\text{CaO}67\text{B}_2\text{O}_3-x\text{Ca}_3\text{WO}_6)$  ( $x = 8-15$  mol%). Additionally, the crystallization of  $\text{CaWO}_4$  was found by Raman spectroscopy due to the formation of  $\text{W=O}$  double bondings of  $\text{WO}_4$  tetrahedra in the pristine glass despite starting with the higher calcium content of  $\text{Ca}_3\text{WO}_6$ . PL/PLE spectra and  $\text{Eu}^{3+}\text{D}_0$  decay curves imply that  $\text{Eu}^{3+}$  ions were excluded from the  $\text{CaWO}_4$  crystals and positioned in the borate glass phase as a stable site for them, which provided local environments in higher symmetry around  $\text{Eu}^{3+}$  ions.

11:10 AM

**(GOMD-S3-006-2022) The role of powder handling on resulting impurities in ZnSe-doped As-S-Se composite materials**

A. Kostogiannes<sup>\*1</sup>; R. Sharma<sup>1</sup>; M. Chazot<sup>1</sup>; M. Kang<sup>1</sup>; C. Blanco<sup>1</sup>; J. Cook<sup>1</sup>; V. Rodriguez<sup>2</sup>; F. Adamietz<sup>2</sup>; D. Verrault<sup>2</sup>; K. Schepler<sup>1</sup>; M. Richardson<sup>1</sup>; K. A. Richardson<sup>1</sup>

1. University of Central Florida, CREOL, USA
2. University Bordeaux, France

The need for mid-infrared (MIR) laser systems capable of emitting in the 3-5 $\mu\text{m}$  spectral region has led to the development of new materials and processing strategies. One of the most promising topics of research is the preparation of composite materials made of divalent transition-metal doped crystals embedded in a chalcogenide glass host. The principal method to prepare such composite materials is by the so-called 'grinding re-melt' process that consists of grinding the components and mixing them before re-melting.

Incorporation of powder processing steps such as grinding, sieving, and mixing can integrate contaminants (most detrimental being O-H, S-H, and Se-H) that produce unwanted absorptions creating optical loss which limits the applicability of novel composite materials. The goal of this study was to investigate and minimize the adverse effects of handling powders for the re-melt technique used in the preparation of ZnSe-doped As-S-Se glass composite materials. We present findings from various steps in powder processing that impact the powder attributes prior to and following melting.

## **S4: Glass Technology and Cross-Cutting Topics**

### **Green Manufacturing**

Room: Constellation F (Second floor)

Session Chairs: Laura Adkins, Corning Research and Development Corporation; Irene Peterson, Corning Incorporated

**9:20 AM**

#### **(GOMD-S4-001-2022) A Review of the Challenges for Melting Reduced Container Glass Colors in Cold Top All-Electric Furnaces (Invited)**

C. P. Ross\*<sup>1</sup>

1. GICI, USA

There is renewed interest in all-electric glass melting as a means of significantly reducing CO<sub>2</sub> emissions. Reduced colors of glass represent more than 50% of all container production. Many past challenges in producing them in all-electric furnaces have not been overcome. This presentation (with a particular focus on Sulfur Redox chemistry) will review past industrial experiences, and which difficulties require more understanding.

**9:50 AM**

#### **(GOMD-S4-002-2022) Hydrogen as a fuel for glass production (Invited)**

O. Verheijen\*<sup>1</sup>

1. CelSian Glass & Solar, Netherlands

Energy-intensive industrial production processes, for example in the glass, food, and ceramic sectors, have a major challenge to decarbonise existing heating processes. A fast and sustainable route to reduce the carbon intensity of these processes is to replace natural gas with hydrogen. Within this presentation the role of hydrogen in the future energy system will be described and potential hydrogen markets will be presented. Furthermore, the state-of-the-art knowledge regarding hydrogen and hydrogen/natural combustion and burner performance will be discussed to allow a gradual transition from natural gas to hydrogen within the glass industry. In addition, the presentation will also address the challenges for the glass industry when applying hydrogen combustion affecting heat transfer, furnace lifetime, and product quality.

**10:20 AM**

#### **(GOMD-S4-003-2022) Furnace of the future, strategies for carbon reduction (Invited)**

E. H. Muijsenberg\*<sup>1</sup>

1. Glass Service, Czechia

With the realities of global warming and plans for CO<sub>2</sub> reduction, the interest in alternative furnace designs such as hybrid electric melting is getting more attention. The generation of electricity by renewable energy sources is, of course, a great help as it brings costs of electricity finally down and will be CO<sub>2</sub> free. In Europe the average generation of electricity by renewable resources is already above 40% coming from wind, solar, hydro and bio. Electricity storage however is complex and expensive, while transporting energy in the form of a gas via pipes is cheaper than via electric wires. An alternative renewable energy carrier is hydrogen. Hydrogen can be generated

via electrolysis using electricity: this conversion, however, is only in the effective range of 65%. After this, hydrogen can be burned in a glass melting furnace with a typical efficiency of 50%. This paper will present Glass Service a.s. (GS) thermal efficiency studies showing if the future will be more likely using electric heating or hydrogen combustion. Results of mathematical modeling show the efficiency of the different technologies. What will be the furnace design of the future?

**10:50 AM**

#### **(GOMD-S4-004-2022) Immersed Radiant Heater - A unique heat source for glass melting (Invited)**

T. Maehara\*<sup>1</sup>; A. Niwa<sup>1</sup>; S. Hyodo<sup>1</sup>; T. Enomoto<sup>1</sup>; T. Yamazaki<sup>1</sup>; Y. Doi<sup>1</sup>; L. Keen<sup>2</sup>; R. Pauli<sup>2</sup>

1. AGC Inc., Innovative Technology Laboratories, Japan
2. Apollo Furnaces Ltd., United Kingdom

With the global demand for CO<sub>2</sub> reduction from the glass melting process, there is growing interest in melting technology using electricity instead of fossil fuel combustion. The most common electric melting technology is a method in which AC is applied between a pair of electrodes inserted in the melt to Joule heat the glass melt itself. In principle, Joule heating requires a large-scale power supply that matches the electrical resistance of the glass melt. Also, glass batches with too high electrical resistance cannot be Joule heated directly. It is an interesting idea to use a radiant heater, which is the heat source of a box-type electric furnace such as that used in a laboratory, to heat a glass melt and even a glass batch in an industrial continuous melting furnace. When such a heat source is realized, the glass melt can be heated by using a generic power supply for a convenient V-A range without any caring about the glass composition. Direct heating of glass batch can also dramatically increase the limited pull rate of cold-top melting. We created a unique heat source for glass melting called the 'Immersed Radiant Heater' and tested the various ideas mentioned above. Then, exciting results that would be a breakthrough for problems of classical electric melting were obtained. In this talk, we will discuss the possibility of new electric melting technology that 'IRH' opens with reference to the test results.

**11:20 AM**

#### **(GOMD-S4-005-2022) Oolitic Aragonite: A Renewable and Sustainable Solution for High Clarity Glass Manufacturing**

A. J. Myers\*<sup>1</sup>

1. Calcean Minerals & Materials LLC, USA

The glass manufacturing industry is under pressure to look for renewable and sustainable raw materials to help meet their sustainability goals. Oolitic aragonite, a unique type of renewable biogenic calcium carbonate that naturally forms on the banks of The Bahamas may be the solution. Oolitic aragonite forms during microbially induced precipitation events called 'whittings' (Robbins & Evans, 1997). The high purity of oolitic aragonite means that it has little to no iron, which is excellent for high clarity glass manufacturing. This paper aims to review peer-reviewed research regarding oolitic aragonite and its sustainability and renewability. More specifically, this paper will discuss the results of a third party verified life cycle analysis (ISO14044:2006) and carbon footprint analysis (ISO14067:2018). Oolitic aragonite was determined to be a carbon negative raw material, meaning it removes more carbon from the atmosphere than the harvesting of aragonite emits. The use of oolitic aragonite in glass manufacturing also helped to reduce global warming potential (GWP) by 18% to 21% compared to the industry average. ASTM D6866 testing also confirmed oolitic aragonite to contain 89% biogenic carbon further supporting its renewability. Oolitic aragonite is an excellent option for glass manufacturers searching for more environmentally conscious raw materials without sacrificing performance.

\*Denotes Presenter



## S1: Fundamentals of the Glassy State

### Mechanical Properties of Glasses: Fracture and Crack Propagation

Room: Frederick (Second floor)

Session Chair: Morten Smedskjaer, Aalborg University

1:20 PM

#### (GOMD-S1-009-2022) Slow Crack Growth in Sodium-Modified Silicate Glasses (Invited)

J. M. Rimsza\*<sup>1</sup>; K. T. Strong<sup>1</sup>; C. Nakakura<sup>1</sup>; J. Duree<sup>1</sup>; K. Stephens<sup>1</sup>; S. Grutzik<sup>1</sup>

1. Sandia National Laboratories, USA

Delayed fracture in silicate glasses is caused by the slow crack growth phenomena, which varies with the glass composition and the environment. Mechanisms of slow crack growth in sodium-modified silicate glasses were evaluated via atomic force microscopy (AFM) and reactive molecular dynamics. Crack velocities in soda-lime silicate glasses were initiated in a bibeam sample in a dry box or an environmental chamber. Crack tip locations were tracked first optically and then using AFM, identifying velocities as low as  $10^{-12}$  m/s with a clear humidity and compositional dependence. Reactive molecular dynamics simulations of fracture in sodium silicate glasses were also performed via far-field loading up to 1.1 MPa $\sqrt{m}$ . The role of sodium content on the mechanisms of crack propagation, including defect and modifier concentration in the inelastic region, surface energy, and the residual stress fields were assessed for their role in causing slow crack growth. Remarkably, stepwise crack propagation was observed in both the AFM data and in the molecular dynamics simulations, though at a different size scale and temporal scales. The propagation and arrest behavior shows some consistency with a transition rate theory of slow crack growth. This study provides the basis for future research into slow crack growth of multicomponent oxide glasses. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 SAND2022-1348A

1:50 PM

#### (GOMD-S1-010-2022) A Comparison of Subcritical Crack Growth Behavior and the Dynamic Fatigue Parameter of Alkali Silicate Glasses

N. Weyrauch\*<sup>1</sup>; R. Brow<sup>1</sup>; K. T. Strong<sup>2</sup>; G. Miller<sup>1</sup>; T. Diebold<sup>2</sup>

1. Missouri University of Science & Technology, Material Science and Engineering, USA
2. Sandia National Laboratories, Material Mechanics and Tribology, USA

Delayed failure in silicate glasses can be linked to subcritical crack growth (SCCG) where surface defects grow over time until catastrophic failure. This phenomenon originates from stress-enhanced chemical interaction between the environment (e.g. water) and the strained silicate crack tip. The SCCG phenomena must be accounted for to predict long term survivability of a silicate glass containing components. This study compares two methods to determine the SCCG parameters for a commercial alkali silicate glass and for a series of binary sodium silicate glasses. The first method utilizes an applied moment double cantilever beam (DCB) to directly measure the three regions of crack velocity ( $v$ ) as a function of stress intensity ( $K_I$ ) to describe SCCG prior to catastrophic failure (Wiederhorn). The second method is based on two-point bend failure strain studies in water on fibers drawn from melts of the same glasses, where the fatigue parameter is obtained by varying the strain rate, and then compared with those obtained from the direct velocity measurements.

2:10 PM

#### (GOMD-S1-011-2022) Origin of Region II Slow Crack Growth of Oxide Glasses

Z. Huang\*<sup>1</sup>; M. Tomozawa<sup>1</sup>

1. Rensselaer Polytechnic Institute, Materials Science & Engineering, USA

Oxide glasses exhibit a slow crack growth behavior in the presence of water vapor. There are three regions in the slow crack growth, region I, region II and region III. There is no consensus regarding to the origin of region II slow crack growth behavior. A new model is proposed that the region II is caused by delayed elasticity, or internal friction, where the elastic modulus of crack tip is transitioned from a high elastic modulus (region III) to a low elastic modulus (region I). This assumption was confirmed experimentally by measuring residual tensile stress after unloading at the end of various stages of slow crack growth by double cleavage drill compression process. After region I, the residual tensile stress field near crack tip, was observed while no such residual stress was observed after region III measurement. This residual tensile stress contour agreed with the calculated tensile stress contour under loading, using the linear elastic fracture mechanics. Besides, the residual tensile stress field near crack tip decayed with time in the same fashion as the stress relaxation process. Finally, the decay (or relaxation) times of the residual tensile stress relaxation at room temperature exhibited a systematic change with the change of water vapor pressure employed for the slow crack growth measurements, with the relaxation time increasing under lower water vapor pressure.

2:30 PM

#### (GOMD-S1-012-2022) Elaboration and fracture properties of glass matrix/glass particles composites

T. Rouxel\*<sup>1</sup>; T. Lacondemine<sup>1</sup>; F. Célarié<sup>1</sup>; P. Houizot<sup>1</sup>

1. Université de Rennes 1, Glass Mechanics, France

A soda-lime-silica glass was used as a matrix to incorporate 7 vol. % of glass beads, about 50  $\mu$ m in diameter, using spark plasma sintering. Three different glass compositions, namely a barium aluminosilicate, a barium-zinc borate and amorphous silica, were selected for the particles, allowing for different elastic and thermal properties. The particles are uniformly dispersed in the matrix and exhibit cohesive bonding to the matrix. The crack path was followed in situ using DCDC specimens and fracture toughness was characterized by the SEPB method. Different toughening mechanisms were observed, including crack deflection, crack branching and crack trapping at particle sites, resulting in a fracture toughness improvement of about 40 %. Poisson's ratios mismatch between the matrix and the particles is found to play a key role.

2:50 PM

#### (GOMD-S1-013-2022) Effect of Local Residual Stress on Fractal Dimension of Silicate Glasses

J. Mecholsky\*<sup>1</sup>; J. Chan<sup>1</sup>

1. University of Florida, Materials Science & Engineering, USA

Local residual stress caused by impacts, machining and indentation results in a decrease in strength in brittle materials. The  $c/r$  ratio for materials without local residual stress has been shown to be constant for a given material and proportional to  $D^*$ , the fractal dimensional increment. The ratio of the critical crack size,  $c$ , and the fracture mirror size,  $r$ , decreases with the existence of local residual stress. However, the global fracture toughness of non-R curve materials is not affected by the local residual stress, and  $D^*$  is directly related to the square of the fracture toughness. We derive a relationship between the fractal dimensional increment and the  $c/r$  ratio for materials fractured with and without local residual stress. We show that the fractal dimension remains constant with the change in the  $c/r$  ratio for local residual stress conditions.



3:30 PM

**(GOMD-S1-014-2022) Residual Stress resulting from ion exchange in silicate glasses (Invited)**G. Macrelli\*<sup>1</sup>

1. Isoclima SpA, R&amp;D, Italy

Ion exchange of alkali in silicate glasses results in the build-up of residual stress. Near-surface compressive stress is beneficial for strength increase. Mathematical models of stress profiles are still challenging mainly because of the complexities of relaxation effects and lack of full understanding of structural behavior of silicate glass under significant, close to yielding conditions, of the spherical and deviatoric components of the stress tensor. Additionally, a full understanding of the interaction of pre-existing and subsequent, in-service-formed surface flaws with residual stress field is still not fully achieved. This last aspect is critical for structural glass applications where strength matters. Notwithstanding this lack of full knowledge ion-exchanged strengthened glass is a product currently used in a number of applications ranging from consumer electronics to structural transportation and architectural constructions. A state-of-the-art discussion is presented from the physical-mathematical modeling phenomenological perspective considering the interrelationship of kinetics with stress and vice versa with consideration for glass's different chemical compositions.

4:00 PM

**(GOMD-S1-015-2022) Fracture Mechanism Analysis of Ultra-Thin Glass for Flexible Display Cover Window**S. Kim\*<sup>1</sup>; W. Chung<sup>2</sup>; G. Shim<sup>1</sup>; S. Jung<sup>1</sup>; H. Sohn<sup>1</sup>; S. Kim<sup>1</sup>

1. Samsung Display Co. Ltd., Republic of Korea
2. Kongju National University, Institute for Rare Metals & Division of Advanced Materials Engineering, Republic of Korea

The worldwide smartphone market has been remarkably grown and reached 1.4 billion units sold in 2021, as embedded technologies and performances of devices have been advanced consistently. Most of all, flexible display devices have shown a huge growth of technology and are expected to take up the main stream of hand-held device markets. By inherent nature of flexible devices, large deformation of all materials, parts and module structures are required in the local or even whole display areas. Since 2020, ultra-thin glass (UTG), less than 50  $\mu\text{m}$  thick, has mostly replaced plastic films to improve picture quality and protection performances from impact loads. In general, UTG cover windows are produced by thickness shaping, cutting, edge finishing, healing, IOX, coating and final inspection. It is indispensable to minimize a flaw size and to maximize foldability and impact resistance in each process. Unfortunately, the mechanism studies of UTG fracture have been rarely carried out due to confidentiality of materials and devices. In this presentation, a fracture mechanism study of UTG in flexible display modules will be introduced. The relationship between the first ring crack and the vertical fracture displacement both by tests and simulations will be verified and suggested. Finally, the development direction and required properties of UTG for future flexible display devices will be briefly introduced.

**S2: Glass and Interactions with Its Environment: Fundamentals and Applications****Dissolution and Interfacial Reactions II: Long-term Corrosion and Nuclear Waste Glasses**

Room: Constellation C/D (Second floor)

Session Chairs: Jon Icenhower, Corning Incorporated; Jincheng Du, University of North Texas

1:20 PM

**(GOMD-S2-015-2022) Long Term Corrosion Interactions between Stainless Steel and International Simple Glass (Invited)**C. Mohanty<sup>1</sup>; X. Guo\*<sup>1</sup>; H. Kaya<sup>2</sup>; S. Gin<sup>3</sup>; K. Yang<sup>4</sup>; Z. Zhang<sup>5</sup>; S. H. Kim<sup>2</sup>; J. Lian<sup>4</sup>; J. Wang<sup>5</sup>; G. Frankel<sup>1</sup>

1. Ohio State University, Materials Science and Engineering, USA
2. Pennsylvania State University, Chemical Engineering and Materials Research Institute, USA
3. CEA, DE2D, France
4. Rensselaer Polytechnic Institute, Mechanical Aerospace and Nuclear Engineering, USA
5. Louisiana State University, Geology and Geophysics, USA

Our recent studies revealed that glass corrosion can be accelerated by the localized corrosion of metals occurring in intimate proximity. Therefore, the long-term corrosion interactions between a simplified nuclear waste glass, international simple glass (ISG), and a candidate metallic canister material, stainless steel (SS) 316L are systematically studied. The experiments were performed by corroding the two materials in 0.6 M NaCl solution at 90 °C for up to one year. Large pits with a diameter exceeding 500  $\mu\text{m}$  were identified on the SS surface, supporting the occurrence of severe localized corrosion. Similarly, localized etching-like corrosion morphology was also observed on the ISG surface, which seems to be associated with the aggressive environment created by the localized corrosion of SS present nearby. Analysis of the leaching solution indicates that the corrosion of glass is highly localized. A parallel experiment was conducted by immersing the same materials in a solution containing 142 ppm dissolved isotopic <sup>29</sup>SiO<sub>2</sub> in addition to 0.6 M NaCl. The results show that the extent of corrosion for both ISG and SS was substantially reduced by the presence of dissolved silica. However, the accelerated corrosion of glass may still be a long-lasting problem since the actual solution in a real repository environment is unlikely to be saturated with silica.

1:50 PM

**(GOMD-S2-016-2022) Applying laboratory methods for durability assessment of vitrified material to archaeological samples**J. Neeway\*<sup>1</sup>; J. Marcial<sup>1</sup>; L. Nava-Farias<sup>1</sup>; C. Pearce<sup>1</sup>; D. Peeler<sup>1</sup>; C. L. Thorpe<sup>2</sup>; C. L. Corkhill<sup>3</sup>; R. J. Hand<sup>2</sup>; D. Kosson<sup>3</sup>; R. Delapp<sup>3</sup>; A. A. Kruger<sup>4</sup>

1. Pacific Northwest National Lab, USA
2. Sheffield University, United Kingdom
3. Vanderbilt University, USA
4. US Department of Energy, USA

Laboratory durability testing used to assess the long-term behavior of nuclear waste forms often involves higher temperature, hydraulically saturated test conditions. However, these accelerated conditions may not be representative of disposal conditions for the nuclear waste form. To address this, we examine vitrified archaeological materials excavated from a ~1500-year old Iron Age Swedish hillfort, Broborg, that have been naturally altered in a near surface environment. We characterized site samples and compared them with corrosion characteristics generated by standard laboratory durability test methods including the product consistency test (PCT), the vapor hydration test (VHT), and the EPA Method 1313

test. Characterization showed limited evidence for natural chemical or physical alteration of the samples from Broborg. Test results show that the altered layer formed on the Broborg samples after VHT displays some similarities to the morphology of the surficial layer formed over longer timescales in the environment. In addition, we use the Arrhenius equation to examine how alteration rates generated in the laboratory tests compare with natural alteration of the samples excavated from Broborg.

### 2:10 PM

#### (GOMD-S2-017-2022) Long-term dissolution of simulated UK Ca/Zn HLW glass in conditions relevant to disposal

M. T. Harrison\*<sup>1</sup>; T. Taylor<sup>1</sup>

1. National Nuclear Laboratory, WM&D, United Kingdom

A new CaZn borosilicate glass formulation for the immobilisation of highly-active Mo-rich waste feeds has been developed in the UK. Non-active lab- and full-scale trials have provided the underpinning to allow deployment this glass on the Vitrification Plant at Sellafield. The demonstration of acceptable product quality to date has used a standard leach test in pure water at high temperatures (90 °C) to compare with the data available for existing UK HLW glass. However, these tests, whilst a useful relative comparison, provide little information about the effect of lower ambient temperatures and the effect of more complex natural groundwaters. Hence, Nuclear Waste Services in the UK is funding a series of durability experiments in conditions more representative of a potential geological repository using the expected range of simulated CaZn glass compositions. These mainly comprise tests for up to 3 years at 40 °C in generic granitic and clay groundwaters as well as de-ionised water at high surface-area-to-volume ratio (1400 m<sup>-1</sup>). SEM-EDS of the leached solids has also been carried out to determine the structure and composition of the alteration layers at the surface. This presentation summarises the full 3-year durability tests, comparing the behaviour of the different CaZn glasses in the three leachant solutions to understand whether composition has a significant effect.

### 2:30 PM

#### (GOMD-S2-018-2022) Insights into the mechanisms controlling the residual corrosion rate of borosilicate glasses

S. Gin\*<sup>1</sup>; X. Guo<sup>2</sup>; J. Delaye<sup>1</sup>; F. Angeli<sup>1</sup>; K. Damodaran<sup>1</sup>; S. H. Kim<sup>3</sup>

1. CEA, DE2D, France
2. Ohio State University, USA
3. Pennsylvania State University, USA

Accurate predictions of glass durability including passivation, require a deep understanding of the mechanisms controlling the so-called residual rate. However, despite tremendous efforts, these mechanisms remain poorly understood. Here, focusing on the behavior of the soluble elements (B, Na, and Ca) of the International Simple Glass, we show that the residual rate is controlled by the behavior of B, a glass former supposed to dissolve instantaneously when in contact with water and thus widely considered as an ideal tracer. We then demonstrate that B release is controlled by multiple processes highly dependent on the pH. At the beginning of the passivating layer formation, the hydrolysis of B-O-Si linkages is rate limiting and has an activation energy of ~60 kJ mol<sup>-1</sup>, a value slightly lower than that for breaking Si-O-Si linkages. Once the fraction of closed pores resulting from gel restructuring is high enough, then diffusion of both reactants (water molecules) and some products (mainly B(aq), Ca(aq)) through the growing gel layer becomes rate-limiting. Consequently, the B and Ca species are trapped in an inner layer referred to as the active zone, with potential feedback on the B-O-Si hydrolysis. A new paradigm, including B as a key element of the system, is proposed to develop a comprehensive model for the corrosion of borosilicate glass.

### 2:50 PM

#### (GOMD-S2-019-2022) Dissolution rate of a simulated nuclear waste glass ISG as a function of solution concentration of Si and pH

Y. Inagaki\*<sup>1</sup>

1. Kyushu University, Department of Applied Quantum Physics & Nuclear Engineering, Japan

Dissolution rate of simulated nuclear waste glass ISG was measured at 70 °C by using Micro-Channel Flow-Through test method as a function of solution concentration of Si at constant pH of 4, 7 and 9, respectively. Si-29 isotope was used for preparing the reaction solution with the Si concentration from 0 to 120ppm in order to distinguish between Si dissolved from glass and Si dissolved in the original solution, and the glass dissolution rate was determined by measuring the dissolution rate of Si-28, major Si isotope (92.2%) of natural Si being consisted of ISG. The test results showed that the glass dissolution rate decreases drastically with an increase of solution concentration of Si at both pH7 and pH9, where the behavior of the glass dissolution rate with solution concentration of Si cannot be accounted by the ordinal first-order dissolution rate law based on SiO<sub>2</sub> dissolution. At pH4, however, the tendency of glass dissolution rate was different from that at pH7 and pH9, where the solution concentration of Si had no remarkable effects on the glass dissolution rate. These results suggested the glass dissolution kinetics change depending on solution pH sensitively.

### 3:30 PM

#### (GOMD-S2-020-2022) Application of the Immobilized Low-Activity Waste Glass Corrosion Model to the Static Dissolution of Enhanced Waste Glasses (Invited)

S. N. Kerisit\*<sup>1</sup>; J. Neeway<sup>2</sup>; C. Lonergan<sup>2</sup>; B. Parruzot<sup>2</sup>; J. V. Crum<sup>2</sup>; J. V. Ryan<sup>2</sup>; M. Asmussen<sup>2</sup>; G. L. Smith<sup>2</sup>

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA
2. Pacific Northwest National Lab, Energy and Environment Directorate, USA

The low-activity waste (LAW) at the Hanford Site will be immobilized through vitrification and disposed of on site at the Integrated Disposal Facility (IDF). The performance assessment (PA) for the IDF analyzes the long-term performance of the planned disposal system, including the release of radionuclides from immobilized low-activity waste (ILAW) glass as predicted by the ILAW glass corrosion model. The most recent IDF PA included an assessment of ILAW glass waste forms that would be produced using the baseline process models at the Hanford Waste Treatment and Immobilization Plant (WTP). However, updated process models have been generated to allow for higher waste loading in ILAW glass formulations, known as enhanced waste glass (EWG). Implementation of the EWG models would greatly expand the expected composition ranges of ILAW glass that could be produced at WTP. This presentation will provide a summary of the application of the ILAW glass corrosion model to simulating the static aqueous dissolution of a statistical matrix of 24 glasses. This glass matrix was defined using contemporary process model constraints and aims to provide coverage of the main components of EWG composition space believe to control glass dissolution. This modeling effort serves to assess the ability of the ILAW glass corrosion model to accurately describe the dissolution of EWG.

**4:00 PM****(GOMD-S2-021-2022) Improvements to the Immobilized Low-Activity Waste Glass Corrosion Model for the Hanford Site Integrated Disposal Facility**

J. Neeway\*<sup>1</sup>; C. Lonergan<sup>1</sup>; S. N. Kerisit<sup>1</sup>; B. Parruzot<sup>1</sup>; J. V. Crum<sup>1</sup>; J. V. Ryan<sup>1</sup>; M. Asmussen<sup>1</sup>; G. L. Smith<sup>1</sup>; D. Swanberg<sup>2</sup>; R. Skeen<sup>2</sup>

1. Pacific Northwest National Lab, USA
2. Washington River Protection Solutions, USA

Immobilized low-activity waste glass will be disposed at the Hanford site Integrated Disposal Facility (IDF). To estimate glass behavior at the IDF, a first-order dissolution rate model for glass is used. The model is comprised of a kinetic portion, which accounts for pH and temperature, and a thermodynamic portion, where the rate is proportional to the activity of orthosilicic acid,  $a(\text{H}_4\text{SiO}_4)$ , with respect to a quasi-equilibrium value,  $K_g$ . The model calculates the long-term glass dissolution rate through a combination of the ion-exchange reaction, represented by a constant release of Na into the system, and through the precipitation of a series of secondary phases. Here, we discuss how the model and the determination of the model parameters have evolved through the years. In addition, we present how model predictions compare with experimental results for a wide range of glass compositions.

**4:20 PM****(GOMD-S2-022-2022) R&D program of operational model of long-term performance for vitrified High-level Radioactive Waste**

R. Matsubara\*<sup>1</sup>

1. Nuclear Waste Management Organization of Japan, Science and Technology Department, Japan

In the Japanese geological disposal program of vitrified High-level Radioactive Waste, the glass matrix is expected to retain radionuclides by limiting radionuclide release into groundwater as an important safety function. Since the performance of vitrified High-level Radioactive Waste depends on thermal, hydraulic, mechanical, and chemical (THMC) conditions, NUMO, as the implementer of geological disposal, has been promoting R&D of operational model for the long-term performance of vitrified High-level Radioactive Waste in consideration of THMC conditions. NUMO has identified R&D issues regarding the glass dissolution and planned the R&D program through FEP (Features, Events, and Processes) analysis and parametric study with numerical model to evaluate relative importance of relevant processes. At present, three R&D programs are ongoing as joint researches with JAEA and two universities: long term glass dissolution experiment to understand evolution of glass dissolution kinetics, glass dissolution experiment at various environmental conditions to assess the performance under several potential repository conditions with the time evolution, and molecular dynamics simulation to understand elemental migration at the interface between glass surface and groundwater. The current status of R&D programs will be introduced in this presentation.

**4:40 PM****(GOMD-S2-023-2022) The impact of Al on the chemical durability of pristine and irradiated borosilicate glasses**

A. Jan<sup>1</sup>; J. Delaye\*<sup>1</sup>; K. Damodaran<sup>1</sup>; S. N. Kerisit<sup>2</sup>; M. Tribet<sup>1</sup>; S. Gin<sup>1</sup>

1. CEA Marcoule, DE2D, France
2. Pacific Northwest National Laboratory, Physical and Computational Sciences Directorate, USA

Pre-irradiated (952 MeV  $^{136}\text{Xe}$  ions) and non-irradiated samples of Na-borosilicate and Na-aluminoborosilicate glasses have been altered during 33 days in a solution enriched with  $^{29}\text{Si}$  and  $^{18}\text{O}$  to understand how gel layer forms and impact the glass dissolution rate. In agreement with atomistic simulations, it has been observed that the initial dissolution rate is larger for the glass without alumina and the protective layer forms more rapidly. In both glasses, the alteration gels are highly enriched in  $^{18}\text{O}$ , but only the alteration layer of

the glass without alumina is enriched in  $^{29}\text{Si}$ . The Al-free glass dissolution occurs through a dissolution – precipitation mechanism while the Al bearing glass dissolution occurs through local hydrolysis and bond reformation. Initial dissolution rates increase by a factor 4 to 6 for irradiated glasses, but surprisingly, at high reaction progress the altered thickness is smaller for the irradiated Al-free glass while it is higher for the irradiated Al-bearing glass. Using Monte Carlo and classical molecular dynamics calculations, explanations are proposed to account for these observations.

**5:00 PM****(GOMD-S2-024-2022) Impact of irradiation on the properties of calcium silicate hydrate (CSH) gel layer formed after aqueous corrosion of borosilicate glasses**

A. Jan\*<sup>1</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, India

Confinement of radionuclides in borosilicate glass matrix is subject to the durability of vitrified nuclear glass in the aqueous medium on the geological time scales under repository conditions. It is now well accepted that under aqueous condition there is a formation of a gel layer. However, the properties of this gel layer are not well understood yet. In this work using atomistic modelling, a series of borosilicate glasses- pristine and irradiated- are prepared and further, gels are prepared by replacing boron and sodium by hydrogen. These gels are then aged at temperature, 2000K. It is seen that, indeed, there is a difference in the properties aged gels (connectivity, short and medium range order) formed from pristine and irradiated glass. Ageing appeared to have a significant effect on the irradiated gels as compared to gels obtained from pristine glasses.

**S3: Optical and Electronic Materials and Devices: Fundamentals and Applications****Glass-based Photonics I: Bulk and Fiber Devices**

Room: Columbia (Second floor)

Session Chairs: Juejun Hu, Massachusetts Institute of Technology; Hongtao Lin, Massachusetts Institute of Technology

**1:20 PM****(GOMD-S3-007-2022) Multicomponent Photonic Glass Fibers and Devices (Invited)**

S. Zhou\*<sup>1</sup>

1. South China University of Technology, School of Materials Science and Engineering, China

In this talk, the recent progress in design, fabrication and application of multicomponent optical glasses and fibers is introduced. First, the typical microstructures in multicomponent glass system represented by topological features, heterogeneities and locally crystallized domains are discussed. Second, the glasses and fibers with various optical functions, including photon generation, amplification, modulation and detection are discussed. Their potential applications as gain matrix of broadband fiber amplifier and advanced probes in optogenetics, femtosecond science and technology, and radiation detection are highlighted.

**1:50 PM****(GOMD-S3-008-2022) Luminescent glass-based materials development for photonics and biophotonics applications (Invited)**

L. Petit\*<sup>1</sup>

1. Tampere University, Finland

Glass-based materials are of interest for the engineering of photonic devices, due to their easy processing. Depending on their composition, they can be engineered with good thermal stability, excellent optical properties and high rare-earth ions solubility. Besides, since



the discovery of the first bioactive glass by Larry Hench, several types of glasses, such as silicates and phosphates, have attracted the attention of many researchers, especially for biomedical applications. However, a major limitation with bioactive glasses is their imaging post-operation as these glass-based materials generally exhibit radiopacity similar to the cortical bone. For the past few decades, in-vivo imaging has been based on fluorescence. Up to now, only few studies that combine both biocompatibility and suitable spectroscopic properties in glasses have been reported. In this presentation, we will review our work on the development of new bioactive glasses suitable for the fabrication of optically active fibers. We will show that it is possible to monitor “in situ” their reaction with the body through changes in the optical properties of the fiber. The study on the development of bioactive composite with persistent luminescence which could be used for in-situ drug delivery will be also presented as well as the first biophotonic composite fiber exhibiting green persistent luminescence.

**2:20 PM**

### **(GOMD-S3-009-2022) Bismuth Borosilicate glass containing Eu<sub>2</sub>O<sub>3</sub> stabilized gold nanoparticles with high third-order nonlinearity**

S. Singla<sup>\*1</sup>; V. G. Achanta<sup>2</sup>; O. P. Pandey<sup>3</sup>; G. Sharma<sup>4</sup>

1. Chandigarh University, Physics Department, India
2. NPL, India
3. Thapar Institution of Engineering & Technology, India
4. KMV College, India

The biggest challenge faced while incorporating metallic-nanoparticles in glass is to control their size, shape, and stability. A new approach to overcome this difficulty is presented here that consists of co-doping of Eu<sub>2</sub>O<sub>3</sub> along with as-prepared gold nanoparticles (GNPs) to prepare GNPs dispersed bismuth borosilicate glass. Eu<sub>2</sub>O<sub>3</sub> forms a covering around GNPs that prevents their loss due to evaporation and coagulation while preparing the glass. The surface plasmon resonance peak position related to GNPs is reported around 585nm. Prepared glass samples are found to be thermally stable and highly suitable for fiber drawing. Intensity-dependent nonlinear behavior of the glass is evidenced by open and closed aperture Z-scan technique from 1.9-14.38 GW/cm<sup>2</sup> range. From open aperture Z-scan data, a switch between saturable absorption to two-photon absorption is observed with the increase in input fluence. A nonlinear refractive index of  $4.7 \times 10^{-18}$  is obtained for GNPs doped samples at a non-resonant wavelength of 800nm.

**2:40 PM**

### **(GOMD-S3-010-2022) Progress towards the development of advanced freeform glass optics**

T. I. Suratwala<sup>\*1</sup>; J. A. Menapace<sup>1</sup>; G. Tham<sup>1</sup>; W. A. Steele<sup>1</sup>; N. Ray<sup>1</sup>; L. L. Wong<sup>1</sup>; B. Bauman<sup>1</sup>

1. Lawrence Livermore National Laboratory, USA

Freeform optics (which are optics with at least one optical surface with no translational or rotational symmetry) are enabling the design of novel optical systems increasing functionality, reduced system size & weight, and reduced the number optical components. As freeform optic designs become more complex, the ability to fabricate them to the design surface figure with the same precision & accuracy as conventional optics (spheres & flats) becomes much more challenging. Here we present recent progress on improving the fabrication of freeform optics by achieving improved determinism in material removal during sub-aperture tool polishing. This includes first developing a comprehensive understanding of the tool influence function (TIF) spot (rotating tool on the glass workpiece), trenches (+ linear translation), and patches (+ overlapping steps). We show that material is removed both by normal and shear load- based material removal mechanisms. Also, the overall TIF shape is influenced by the spatial and temporal velocity distribution, a combined elastic mechanics & hydrodynamic pressure distribution, spatially dependent friction coefficient, and workpiece curvature. In addition, a detailed

understanding of mid-spatial frequency errors (which are inherently created during sub-aperture tool polishing) are described with novel design rules to minimize them via control of tool process parameters.

## **Glass-based Photonics II: Planar Devices**

Room: Columbia (Second floor)

Session Chairs: Hongtao Lin, Massachusetts Institute of Technology; Juejun Hu, Massachusetts Institute of Technology

**3:20 PM**

### **(GOMD-S3-011-2022) Self-assembled chalcogenide photonic integrated circuits on silicon (Invited)**

W. Shi<sup>\*1</sup>; P. Jean<sup>1</sup>; A. Douaud<sup>2</sup>; S. Laroche<sup>1</sup>; Y. Messaddeq<sup>2</sup>

1. Université Laval, Department of Electrical and Computer Engineering, Canada
2. Université Laval, Center for Optics, Photonics, and Lasers, Canada

Chalcogenide glasses have exceptional optical properties in the infrared region. Spontaneous matter reorganization of chalcogenide thin films through the dewetting process provides a way for etch-less self-assembled optical waveguides. Using this approach, we integrate chalcogenide onto a pre-processed silicon photonic chip and show that the use of pre-patterned templates leads to organized, reproducible patterns with large-scale uniformity of chalcogenide waveguide structures. We achieved compact chalcogenide micro-resonators directly coupled to silicon waveguides, showing a 4.7 million quality factor and a 0.08 dB/cm waveguide propagation loss. Heterogeneous integration of chalcogenide and silicon photonic waveguides allows combination of advantages of the two material platforms for novel functions such as athermal photonic integrated circuits and Raman-Kerr combs.

**3:50 PM**

### **(GOMD-S3-012-2022) Phase change material enabled parafocal zoom metalens**

J. Hu<sup>\*1</sup>

1. Massachusetts Institute of Technology, USA

Zoom lenses with variable magnification ratios are essential for many optical imaging applications. Conventional zoom lenses are composed of multiple refractive optics, and optical zoom is attained via translational motion of one or more lens elements, which adds to module size, complexity, and cost. In this talk, we present a zoom lens design based on multi-functional optical metasurfaces which achieves large step zoom ratios, minimal distortion and diffraction-limited optical quality without requiring mechanical moving parts. A zoom metalens based on a low-loss phase change materials Ge<sub>2</sub>Sb<sub>2</sub>Se<sub>4</sub>Te (GSST) was experimentally demonstrated in the mid-infrared, achieving 10x parafocal zoom with negligible distortion in accordance with our design.

**4:10 PM**

### **(GOMD-S3-013-2022) Phase change material based metasurfaces on a foundry-processed silicon-on-insulator platform**

C. Popescu<sup>\*1</sup>; Y. Zhang<sup>1</sup>; C. Ríos<sup>2</sup>; Q. Du<sup>1</sup>; L. Martin-Monier<sup>1</sup>; L. Ranno<sup>1</sup>; M. Shalaginov<sup>1</sup>; P. Miller<sup>3</sup>; C. Roberts<sup>3</sup>; M. Kang<sup>4</sup>; K. A. Richardson<sup>4</sup>; T. Gu<sup>1</sup>; S. Vitale<sup>3</sup>; J. Hu<sup>1</sup>

1. Massachusetts Institute of Technology, Department of Materials Science and Engineering, USA
2. University of Maryland, Department of Materials Science and Engineering, USA
3. Massachusetts Institute of Technology, Lincoln Laboratory, USA
4. University of Central Florida, The College of Optics and Photonics, Department of Materials Science and Engineering, USA

Chalcogenide phase change materials (PCMs) have been in industrial use such as CDs and DVDs for decades due to their large change in refractive index upon amorphous-crystalline phase transition. They are finding new applications in integrated photonic circuits,



neuromorphic computing, active metamaterials/metasurfaces, and more. Metasurfaces leverage the geometry of subwavelength nano-antennae to modulate the incoming light signal and PCM-based ones allow for added flexibility in optical applications. Electric pulse heating is a method of switching PCMs that is amenable for use in integrated circuits over furnace annealing or laser heating. Here, we present recent work on using doped silicon-on-insulator (SOI) heaters to switch metasurfaces made out of  $\text{Ge}_2\text{Sb}_2\text{Se}_4\text{Te}$ , a low loss PCM in the telecom range. The SOI platform presents the possibility of transmissive active integrated optical devices in the near-IR.

#### 4:30 PM

##### (GOMD-S3-014-2022) Flexible glass integrated photonic devices with superior optical and mechanical performance

Y. Luo<sup>\*1</sup>; C. Sun<sup>1</sup>; H. Ma<sup>2</sup>; M. Wei<sup>2</sup>; J. Li<sup>2</sup>; J. Jian<sup>1</sup>; C. Zhong<sup>2</sup>; Z. Chen<sup>1</sup>; R. Tang<sup>1</sup>; K. A. Richardson<sup>3</sup>; H. Lin<sup>2</sup>; L. Li<sup>1</sup>

1. Westlake University, School of Engineering, China
2. Zhejiang University, College of Information Science and Electronic Engineering, China
3. University of Central Florida, Department of Materials Science & Engineering, USA

Chalcogenide glass photonic integration on thin flexible plastic substrates is a rapidly emerging technology with a wide range of possible applications in the fields of flexible optical interconnects, conformal sensing, health monitoring, and biotechnology. In this work, we designed and fabricated several flexible passive devices based on a combination of a monolithic integration technique and the multi-neutral axis theory. The microring resonator, waveguide crossing, multimode interferometer, and Mach-Zehnder interferometer were demonstrated at 1.55  $\mu\text{m}$  with superior optical and mechanical performance. In addition, a flexible side-coupled Bragg-grating-assisted Fabry-Perot filter was also constructed to achieve only one dip within a broad wavelength range covering the whole S+C+L band, which could be applied as the basic sensing unit for the mapping of mechanical properties in 3D space. These results represent a significant step towards the potential application of a flexible photonic integrated circuit.

#### Optical and Photonic Glasses and Glass-ceramics II

Room: Constellation E (Second floor)

Session Chair: Russell Leonard, University of Tennessee Space Institute

#### 1:20 PM

##### (GOMD-S3-015-2022) Waveguides based on germanate and tellurite glasses fabricated with Si technology and fs laser writing techniques for IR applications: A review (Invited)

L. R. Kassab<sup>\*1</sup>

1. Faculty of Technology of Sao Paulo, Departamento de Ensino Geral, Brazil

The search for new materials doped with rare earth ions and metallic nanoparticles has grown due to several applications. In particular  $\text{GeO}_2\text{-PbO}$  and  $\text{TeO}_2\text{-ZnO}$  glasses appear as potential candidate for photonics: they have linear and nonlinear refractive index, wide transmission window (400-500nm) and low cutoff phonon energy with respect to silicates; photoluminescence enhancement due to localized plasmon effects was also demonstrated in these hosts as well as nonlinear optical properties. We review different pedestal waveguides with rare earth ions doped  $\text{GeO}_2\text{-PbO}$  cores and decorated with gold nanoparticles for applications at the IR. The Silicon technology used to fabricate the pedestal, followed by core material deposition with the sputtering technique are presented. The

advantages of pedestal architecture with respect to rib waveguides are discussed and the advances that led to the waveguides optical improvement regarding propagation losses and relative gain. Results of waveguides written directly in the same glasses using the fs laser writing for the production of a new double line architecture are also shown. The present results open new possibilities for integrated photonics

#### 1:50 PM

##### (GOMD-S3-016-2022) Effect of UV exposure and low temperature treatment on optical properties of Photo-Thermo-Refractive glass

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2. Optigrate Corp., USA

Photo-Thermo-Refractive (PTR) glass is a photosensitive material for volume holographic Bragg gratings (VBG) recording. The VBG fabrication process includes irradiation of glass (recording), and thermal aging above glass transition temperature (470°C). However, there is no information about temperature when structural transformations in PTR glass started. This is why structural changes after heat treatment below glass transition temperature were studied by analyzing absorption, photoluminescence, and scattering. Virgin, irradiated, and treated at 300, 350, 400 and 450°C samples were studied. Irradiated and heat treated on 300, 350, 400°C samples have been shown the induced absorption band at 360 nm. Heat treated samples on 350, 400 and 450°C have been shown the increasing of absorption in the visible part. Photoluminescence measurements showed that for virgin and UV-exposed samples excited at 360 nm an emission band around 430 nm appears. Photoluminescence bands with excitation at 360 and emission at 480 nm, excitation on 460 nm and 550 nm and emission on 700 nm, for thermally treated samples were detected. No emission maximum on 480 nm was observed for sample treated at 450 °C. The scattering measurements showed no difference for all the measured samples. It was concluded that structural transformations occurring at these conditions take place only at atomic scales.

#### 2:10 PM

##### (GOMD-S3-017-2022) Ultraviolet Opacification of Ce-Mn Codoped Silicate Glass

C. Bellows<sup>\*1</sup>; A. G. Clare<sup>1</sup>

1. Alfred University, USA

Typical opacification of glass presents as broad spectrum and is not easily altered without subsequent heat treatments. However, the combination of cerium and manganese ions in a standard soda-lime-silicate glass composition exhibits a novel optical effect: luminescent opacity. Under visible light illumination, this composition appears transparent purple; similar to other silicates containing the  $\text{Mn}^{3+}$  ion. As with other silicates doped with  $\text{Ce}^{3+}$  and  $\text{Mn}^{2+}$  ions, this composition also luminesces visible light under ultraviolet light. Yet, unlike similar compositions, under said ultraviolet light the glass acquires a certain turbidity not seen under visible light. Interestingly, when the ultraviolet source is removed, the glass returns to a transparent purple rather than maintaining its opacity. Through a combination of spectroscopic techniques and microscopic imaging, an attempt to ascertain the cause of this simultaneous luminescence and opacification is made.

2:30 PM

### (GOMD-S3-018-2022) 2D and 3D Structural Evolution and Chemical Characterization of Nanoparticles in Fiber Optics

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1. Thermo Fisher Scientific, Materials and Structural Analysis Division, USA
2. Harvard Medical School/Brigham and Women's Hospital, USA
3. CAMECA, USA
4. Clemson University, USA
5. University of Bordeaux, France
6. Institut de Physique de Nice, France

The doping of optical fibers with nanoparticles (NP) has been of growing interest in recent years, in particular for the development of new fiber lasers or amplifiers, by engineering the luminescence properties of rare earth ions. A particularly promising recent application concerns the production of sensors (temperature, stress, chemical, etc.) based on light backscattering. Those exciting applications are highly dependent on our ability to control and measure the size and properties of NP. Since we have previously reported that NP formed via phase-separation mechanisms do exhibit a size-dependent composition, we shifted our focus on another approach, based on doping the core of a silica-based optical fiber with  $\text{LaF}_3:\text{Tm}^{3+}$  NP. We can demonstrate that although characterizing those NP presents technical challenges, an analytical workflow involving focused-ion beam (FIB) sample preparation, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and x-ray microanalysis, provides great insights to glass scientists. Indeed, our experimental results revealed a strong link between composition and size of the NP, irrespective of the doping process. This has a significant impact, especially for laser and amplifier applications that target small-sized NP.

2:50 PM

### (GOMD-S3-019-2022) Atomistic Simulation Study of Li-Aluminosilicate Glass Scintillators

E. Ghardi<sup>\*1</sup>

1. Bangor University, Nuclear Future Institute, United Kingdom

Radiation sensors are an important enabling technology in a number of fields, such as medicine, research, energy, military and homeland security. Glass base scintillators have been in use for more than 50 years and offer some benefits including their ability to respond to different types of radiation, and to be formed into various shapes. There is, however the possibility to discover and improve glass scintillators. With this in mind, this work provides insight from atomic scale simulations on the cerium doped Li-Aluminosilicate ( $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-MgO-Li}_2\text{O-Ce}_2\text{O}_3$ ) glass scintillators. Three glass compositions were studied using Molecular Dynamics (MD) and Density functional Theory (DFT) to investigate the effect of the ratio (with  $R = [0.3, 0.8 \text{ and } 2]$ ) on structural, electronic and optical properties. The effect of  $R$  on the complex structure of the system of interest was mainly associated to the increase of  $Q_4$  population that replaced  $Q_3$ 's within the network, while electronic mid gap defects were found to be present when  $R < 1$ . The optical properties including absorption coefficients and energy loss spectra are calculated and analysed based on the electronic structures.

3:10 PM

### (GOMD-S3-020-2022) Glasses for multiband visible/IR optics

D. Gibson<sup>3</sup>; W. Kim<sup>\*1</sup>; V. Nguyen<sup>1</sup>; K. Major<sup>2</sup>; A. Floyd<sup>4</sup>; S. Bayya<sup>3</sup>; J. Sanghera<sup>1</sup>

1. U.S. Naval Research Laboratory, Optical Sciences Division, Code 5621, USA
2. US Naval Research Laboratory, Optical Sciences Division - Code 5623, USA
3. US Naval Research Laboratory, Optical Sciences Division - Code 5622, USA
4. Jacobs, On-site contractor for NRL Code 5622, USA

Recent developments in wideband focal plane arrays offers an opportunity for extended wavelength imaging but is hindered by the limited catalog of refractive materials capable of multiband

operation. This paper presents efforts to expand the glass map for optical systems tasked with simultaneous imaging in visible and mid-wave infrared (out to about 5  $\mu\text{m}$ ) wavebands through development of new oxide glasses and glasses for other important IR wavebands. The impact of chemistry and processing on glass structure and properties will be explored with an emphasis on defense applications.

## S4: Glass Technology and Cross-Cutting Topics

### Forming and Coatings

Room: Constellation F (Second floor)

Session Chairs: Jennifer Rygel, Corning Incorporated; Irene Peterson, Corning Incorporated

1:20 PM

### (GOMD-S4-006-2022) Scalable Deposition of Durable Antimicrobial Thin Film Coatings on Complex Shaped Glass Substrates (Invited)

I. Sokmen<sup>\*1</sup>; B. Okan<sup>1</sup>; H. Erdem<sup>1</sup>; R. Budakoğlu<sup>1</sup>; G. Aydin<sup>1</sup>; Z. Aydin<sup>1</sup>; A. Özen<sup>1</sup>

1. Türkiye Sise ve Cam Fabrikalari A.S., Science Technology and Design Center, Turkey

COVID19 global pandemic forces the glass industry to reposition itself because pristine glass surface is a forgiving host for microorganisms. Bacteria and viruses can survive for long durations on untreated glass surfaces thereby facilitating transmission. Despite the availability of several antimicrobial-coating treatments, glass industry is also bound with fundamental production constraints, which severely limit the applicative range of such treatments. The standing challenges include the need to preserve the optical characteristics of the treated articles, need for a scalable and cost-effective deposition technology, cost effectiveness, and meeting of extensive chemical/mechanical durability requirements. This talk is focused on V-block antimicrobial thin film coating development at Sisecam. V-block is a nanometer thick inorganic coating that bears transition metal doped oxide semiconductor chemistry deposited with atmospheric chemical vapor deposition techniques. This deposition method is well suited for coating complex shaped articles and accommodate high line speeds and high temperature gradients observed on the glass surface. It will also be discussed performance characteristics of V-block coating system in reference to antimicrobial test protocols, possible sources of antimicrobial activity, thin film optical properties and durability characteristics.

1:50 PM

### (GOMD-S4-007-2022) Latest Development in Hot Forming of 3D Shaped Thin Glass Components for Mass Production

P. Vogel<sup>\*1</sup>; A. Vu<sup>1</sup>; C. Strobl<sup>1</sup>; T. Grunwald<sup>1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer Institute for Production Technology IPT, Fine Machining and Optics, Germany
2. Laboratory for Machine Tools WZL RWTH Aachen University, Germany

The constantly developing market for complex 3D shaped thin glass is determined by applications in the automotive and consumer electronics sectors. Important applications are, for example, cover glasses for smartphones and for the car interiors such as center consoles or Head-Up Displays, as well as components for optical systems. These applications share comparable requirements in terms of shape complexity, form accuracy and product variation with simultaneously rising pressure for cost reduction. Direct manufacturing processes such as grinding and polishing fail to meet the cost requirement due to low scalability and are limited when machining thin glass because of an increased fracture risk. At Fraunhofer IPT, hot forming of thin glass has been developed and has become a viable technological solution to the aforementioned problems. In particular, so-called non-isothermal processes, in which heating of

glass and mold tools is separated, permits the shortest possible mold occupation time and highest efficiency leading however to complex heat transfer mechanism. This presentation aims to introduce the key factors to achieve a successful process of thin glass forming. Furthermore, the latest development in process enhancement and machine technology (consisting of experimental, simulation based or machine learning methodologies) will be discussed providing application orientated guidelines.

### 2:10 PM

#### (GOMD-S4-009-2022) Enabling energy- and cost-efficient production of glass optics by non-isothermal wafer-level glass molding

C. Strobl<sup>\*1</sup>; P. Vogel<sup>1</sup>; A. Vu<sup>1</sup>; T. Grunwald<sup>1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer Institute for Production Technology, Fine Machining and Optics, Germany
2. RWTH Aachen University, Laboratory for Machine Tools WZL, Germany

Non-isothermal glass molding has become a viable hot forming technology for mass production of optics. Numerous optic applications are promising from lighting and projection optics for modern vehicles to home or street lighting using LED technology. The major challenge is an enabling scalable replication process allowing the molded glass units with high form accuracy and at low-cost production. This presentation aims at the introduction of our recent development concerning the non-isothermal hot forming on wafer-scale. While addressing the above mentioned requirements, new challenges arise. Besides the selection of suitable mold concepts and materials, these challenges also include the temperature control of the mold and the blank up to the optimization of flow and shrinking mechanisms of the glass during rapid forming. Furthermore, general technical problems of non-isothermal glass molding such as form accuracy, repeatability, and process optimization will be discussed in depth. Finally, detail calculations of cost and energy consumption, in comparison with conventional fabrication of glass components using grinding and polishing, will be demonstrated. The non-isothermal wafer-level molding promises a new technological platform for the manufacturing of optics at large-scaled production.

### 2:30 PM

#### (GOMD-S4-010-2022) Monte-Carlo simulation based wear prediction for Precision Glass Molding of fused silica

T. Grunwald<sup>\*1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer IPT, Fine Machining and Optics, Germany
2. WZL Tool Machine Laboratory of RWTH Aachen University, Chair for Manufacturing Technology, Germany

Fused silica as a highly durable optical material for laser beam shaping or optical communication plays an irreplaceable role in the future of photonics. The conventional, direct manufacturing processes for the production of fused silica optics (e.g. grinding and polishing) are increasingly reaching the limits of efficiency and complexity (scalability of production or production of complex geometries). The Precision Glass Molding of fused silica can overcome these limits, but faces challenges that prevent it from becoming a significant industrial application. These include primarily the wear of the molding tools, which is caused by the challenging process conditions (temperatures of up to 1,400 °C, high forming stresses, etc.). Although the mold wear mechanisms are well understood in a qualitative sense, quantitative service lifetime prediction for the forming process cannot be provided. This study presents a mathematical model comprising a combined Monte-Carlo and Multi-objective genetic algorithm approach in order to overcome this issue. The simulation is able to reproduce the dynamic surface alteration during the wear occurrence. The explanations close with an outlook concerning the transferability of the simulation to other issues in glass and manufacturing science.

### Glass Challenges

Room: Constellation F (Second floor)

Session Chairs: Jennifer Rygel, Corning Incorporated; Irene Peterson, Corning Incorporated

### 3:40 PM

#### (GOMD-S4-012-2022) Conference on Glass Problems – Sharing Glass Manufacturing Innovations and Educating the Next Generation of Glass Engineers

S. K. Sundaram<sup>\*1</sup>; R. Lipetz<sup>2</sup>

1. Alfred University, Inamori School of Engineering, USA
2. Glass Manufacturing Industry Council, USA

Conference on Glass Problems has been bringing together glass manufacturers, raw materials suppliers, and equipment makers over the past 83 years. It is the largest glass manufacturing conference in North America, attracting glass manufacturers and suppliers worldwide to exchange innovations and problem solutions. Co-organized by the Glass Manufacturing Industry Council and Alfred University, the conference provides expert lectures, panel discussions and focused courses and symposia, along with exhibiting and networking opportunities. An advisory board with members representing the glass manufacturing industry assembles the technical program covering two full days annually. Plenary lectures by experts from the industry highlights current problems and innovations. This is followed by contributed presentations from a wide range of problem solvers from the glass manufacturing industry. In addition, undergraduate and graduate students are supported with travel stipends and encouraged to attend. The Conference includes industrial exhibits. This lecture surveys some of the most significant lectures over the past decade, highlighting issues and technology innovations that have shaped the industry over the years.

### 4:00 PM

#### (GOMD-S4-013-2022) GlassArtEngine – Teaching Across Glass Arts, Science, and Engineering

C. Bellows<sup>1</sup>; E. M. Tsekrekas<sup>1</sup>; D. Möncke<sup>\*1</sup>; A. G. Clare<sup>1</sup>; S. K. Sundaram<sup>1</sup>; A. Powers<sup>2</sup>

1. Alfred University, Inamori School of Engineering, USA
2. Alfred University, School of Arts and Design, USA

We present our experience and success with teaching across disciplines of art and engineering, GlassArtEngine, at Alfred University over the past ten years. The team includes professors and graduate students as teaching assistants from glass arts and glass engineering science programs. The curriculum has been shaped over the past decade with yearly feedback from the students, faculty, and community members. The unique revolutionary pedagogy involves active participation and experiential learning of students and team efforts culminating in a joint exhibition at the end of the semester. At the beginning of the course, the students are asked to express their expectations and aspirations for the course over short presentations to the class. Quick tours of laboratories, studios, and other spaces within the schools are given. This is followed by short presentations by faculty about various aspects of glass art, current scientific research topics, and broad themes. Teams are then formed along various themes and allowed to work as a team with flexible time to manage ideation and execution. A mid-term mini exhibit is evaluated and critiqued to provide inputs that are critical to the final exhibition. An overview our approach and results along with examples will be presented.



## Poster Session

Room: Atrium/Harborview (Second floor)

6:30 PM

### (GOMD-S1-SP001-2022) Impact of a Temperature-Dependent Stretching Exponent on Glass Relaxation

B. Hauke<sup>\*1</sup>; M. Mancini<sup>1</sup>; J. C. Mauro<sup>1</sup>

1. Pennsylvania State University, MatSE, USA

The nonexponential relaxation behavior of glass is governed by the dimensionless stretching exponent,  $\beta$ , which is typically assumed to be a constant but is more accurately described as a function of temperature. Relaxation calculations of glassy materials are undertaken via an iterative differential equation-based algorithm to determine when the use of a temperature-dependent (or dynamic) stretching exponent is required to capture the industrially relevant evolution of fictive temperature components, which is necessary for process engineering. Results reveal a range of liquid fragility index ( $m$ ) in which a static  $\beta$  description is roughly equivalent to the behavior observed with a dynamic  $\beta$ . However, fast primary ( $\alpha$ ) relaxation modes demonstrate unique behavior in systems exhibiting excessively strong or fragile liquid behavior when a temperature-dependent stretching exponent is considered.

### (GOMD-S1-SP002-2022) Dynamic Light Scattering in Potassium Borate Glass Melts

H. Uppala<sup>\*1</sup>; D. Sidebottom<sup>1</sup>

1. Creighton University, Physics, USA

We report dynamic light scattering measurements performed on potassium borate glass melts at temperatures near the glass transition. Borate glass melts provide a platform to study structural effects on fragility and non-exponentiality, given their ability to vary their bond density when alkali is added to the mixture. Photon correlation spectroscopy was performed on boron oxide melts doped with 0-10% potassium oxide by mole fraction. This data provides insight into the dynamic structure factor of liquid and the  $\alpha$ -relaxation, from which both fragility and non-exponentiality can be characterized. Two relaxations were observed, the first of which we attribute to be the viscoelastic  $\alpha$ -relaxation, typical of most liquids, while the second we attribute to potassium ion diffusion within the glass melt.

### (GOMD-S1-SP003-2022) NMR Investigations of the Structural Role of Phosphorous in Aluminosilicate Glasses for Ion Exchange

A. Cowen<sup>\*1</sup>; M. Bovee<sup>2</sup>; D. Srivastava<sup>2</sup>; J. Wu<sup>3</sup>; P. J. Grandinetti<sup>2</sup>

1. Ohio State University, Materials Science and Engineering, USA
2. Ohio State University, Department of Chemistry, USA
3. Corning Incorporated, Glass Research, USA

Chemically strengthened aluminosilicate glasses are used in applications from phone screens to airplane windshields, where the consequences of flaws can range from inconvenient to disastrous. The addition of phosphorous to these glasses depolymerizes the network and promotes ion exchange, creating stronger glasses in less time. Thus, understanding the role of phosphorus in the structure is necessary to design glasses that optimize the strengthening process. While previous  $^{31}\text{P}$  magic-angle spinning (MAS) nuclear magnetic resonance (NMR) investigations of these glass compositions reveal significant variations in local structure around  $\text{PO}_4$  species, the MAS spectra contain many strongly overlapping resonance, making assignments and quantification challenging, if not impossible. In this work, we employ two-dimensional  $^{31}\text{P}$  magic angle flipping (MAF) NMR measurement, which correlates the isotropic MAS spectrum to the off-magic angle ( $90^\circ$ ) spectrum, to reveal details on the identity and quantification of phosphorus site speciation. Our investigation focuses on a series of aluminosilicate glasses  $0.20 \text{ K}_2\text{O} \cdot 0.20 \text{ Al}_2\text{O}_3 \cdot 0.60 \text{ SiO}_2$  and  $0.20 \text{ Na}_2\text{O} \cdot 0.20 \text{ Al}_2\text{O}_3 \cdot 0.60 \text{ SiO}_2$  perturbed by the addition of 0 to 10 mol%  $\text{P}_2\text{O}_5$ . To aid in our spectral

interpretation, we have performed quantum chemistry calculations of the  $^{31}\text{P}$  nuclear shielding tensors on clusters modeling local structure around  $\text{PO}_4$  species.

### (GOMD-S1-SP004-2022) Alkali Tungsten-Borate: Investigation of Structure and Properties

E. M. Tsekrekas<sup>\*1</sup>; A. G. Clare<sup>1</sup>

1. Alfred University, Glass Science, USA

Heavy metal transition metal ions are often used as “probes” to determine the elementary structural units within a glass. When concentrations reach above the dopant level, many these transition metals also exhibit behaviors of a conditional glass former, being able to participate in the glass network either as a modifier or the glass former itself. Tungsten-based glasses are of particular interest because they exhibit excellent photochromic and electrochromic properties along with being structurally diverse. This study investigates a series of alkali-tungsten borate glasses to better understand the composition-structure-property relationships of these glasses to better tailor glasses for real world applications. Glass structural studies were done using Raman spectroscopy to identify borate and tungstate units within the network. In addition, physical, thermal, and optical properties were measured.

### (GOMD-S1-SP005-2022) Oxygen Triclusters and Five-Coordinated Alumina Species in Calcium-aluminosilicate Glasses

S. Astle<sup>\*1</sup>; R. Welch<sup>1</sup>; J. C. Mauro<sup>1</sup>

1. Pennsylvania State University, Materials Science and Engineering, USA

Calcium aluminosilicate glasses are technologically important for liquid displays and other optical devices. Despite their presence in industrially relevant applications, the short-range structure for this glass system is widely debated. This work explores the formation of debated structural units such as oxygen triclusters and five-coordinated alumina species. Molecular dynamics was used to study various compositions at different liquidus temperatures to understand how thermodynamics and kinetics impact the formation of such species. Results show a formation of oxygen triclusters with limited five-coordinated alumina despite what is expected experimentally. A preliminary statistical mechanics model was applied to the system to predict the formation of structural units for any given composition within the glass system.

### (GOMD-S1-SP006-2022) Untypical blue colors in glasses with varying optical basicity

L. Greiner<sup>\*1</sup>; J. Kasprzyk<sup>1</sup>; D. Möncke<sup>1</sup>

1. Alfred University, Glass, USA

Soda-lime-silicate glasses are known to exhibit a deep blue color when doped with Cobalt ( $\text{Co}^{2+}$ ), or sky-blue color when doped with divalent  $\text{Cu}^{2+}$  or  $\text{Fe}^{2+}$ . Weak blue  $\text{W}^{5+}$  and  $\text{Nb}^{4+}$  have also been reported in reduced melted phosphate glasses. However, high basicity glasses can turn corn-flower blue when containing less usual oxidation states of Nickel ( $\text{Ni}^{3+}$ ), turquoise when containing Manganese ( $\text{Mn}^{5+}$ ), or blue when Titanium is reduced to ( $\text{Ti}^{3+}$ ) in tetrahedral coordination. Even Sulfur can form a deep blue ultramarine as known from Lapis lazuli. The latter is an anion-to-anion charge transfer transition within  $\text{S}_3^-$  clusters, while the optical spectra of the earlier listed dissolution colors can be interpreted by ligand field theory. Ligand field strength and Racah parameters were deduced from the optical spectra and related to the optical basicity of the different samples, which ranged from phosphate to meta-silicate glasses. The electronic configuration, coordination, and oxidation states are discussed.



**(GOMD-S1-SP008-2022) Structural Evidence of Mixed Alkali Effect for Aluminoborosilicate Glasses**S. Hyun\*<sup>1</sup>; J. Cho<sup>1</sup>

1. Pohang University of Science and Technology (POSTECH), Ferrous Technology, Republic of Korea

The structure of mixed alkali aluminoborosilicate is quite difficult to explain due to the mixed alkali effect and interaction between multiple network formers, intermediate oxides, and network modifiers. To understand the complex behavior of these components in mixed alkali glasses, solid-state MAS NMR and Raman spectroscopy were performed. Various Raman peaks were specifically revealed, and all of which were highly associated with the degree of polymerization (DP) obtained by deconvolution of 800-1200  $\text{cm}^{-1}$ . A systematic change of the glass network was well explained to be a consequence of a strong relationship between DP and MAS NMR results of network formers ( $^{27}\text{Al}$  and  $^{11}\text{B}$ ). When alkali cations were mixed, a new characteristic of mixed alkali effect, an increase in charge compensation stability between  $\text{AlO}_4$  and smaller cation, was first observed from high correlation between full width at half maximum (FWHM) of network modifiers ( $^7\text{Li}$  and  $^{23}\text{Na}$ ) and MAS NMR data of network formers.

**(GOMD-S1-SP009-2022) A two-point bending study of the failure characteristics of ion-exchanged glass fibers**T. C. Lewis\*<sup>1</sup>; R. Brow<sup>1</sup>; D. Thien<sup>1</sup>

1. Missouri University of Science & Technology, Materials Science and Engineering, USA

Glass fibers about 100 microns in diameter were pulled from melts of a sodium aluminosilicate glass and their failure strains were measured using the two-point bending (2pb) technique, before and after ion-exchange treatments in molten  $\text{KNO}_3$ . The 2pb measurements were done in room temperature air with different relative humidity and were done at different faceplate velocities to characterize fatigue sensitivity. Pristine fibers have failure strains and fatigue parameters similar to other aluminosilicate glasses, whereas the failure strains of ion-exchanged fibers were generally lower than the pristine fibers, whereas the fatigue parameters were greater. Ion exchanged fibers were characterized by IR and Raman spectroscopies and scanning electron microscopy, and the resulting information is used to explain the trends in failure strains.

**(GOMD-S1-SP010-2022) Water as a flux in a hybrid coordination network glass**S. S. Sørensen\*<sup>1</sup>; X. Ren<sup>1</sup>; T. Du<sup>1</sup>; L. R. Jensen<sup>2</sup>; M. M. Smedskjaer<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Aalborg University, Department of Materials and Production, Denmark

Hybrid coordination network (HCN) glasses, including for example metal-organic framework glasses, consist of metal ion nodes connected by organic linkers through coordination bonds, in many cases resembling the short-range structure encountered in oxide glasses. However, while the properties of oxide glasses may be significantly changed by adding so-called network modifiers, i.e., metal oxides which break up the interpenetrating network by creating non-bridging oxygens, this phenomenon has not yet been observed in HCN glasses. Here, we present evidence for water acting as a flux or "modifier" in a HCN glass. Specifically, upon water addition to the parent crystal, the melting and glass transition temperatures decrease, before reaching a constant value at high water content. We investigate the water-facilitated melting and glass-formation mechanism by calorimetry, spectroscopy, and ab initio simulations, showing how water is incorporated into the network structure and its effect on the measured thermal properties. Our work sheds light on how some HCN glasses mimic the flux behavior of oxides, providing an important path for tuning their glass formation propensity and resulting material properties.

**(GOMD-S1-SP011-2022) FTIR study on nanoceria created and extracted from a soluble sodium borate glass**K. S. Ranasinghe<sup>2</sup>; A. Vasquez\*<sup>1</sup>; R. Singh<sup>1</sup>

1. Kennesaw State University, Chemistry and Biochemistry, USA
2. Kennesaw State University, Physics, USA

Cerium Oxide nanoparticles have been of interest for many years due to its possible applications as an antioxidant that give it properties to scavenge toxic radicals found in neurodegenerative diseases, Cancer, Alzheimer's, and inflammatory conditions. What gives Cerium Oxide nanoparticles their antioxidant property is the coexistence of  $\text{Ce}^{3+}$  and  $\text{Ce}^{4+}$ . Cerium has two partially filled subshells that allow for several excited states. Our research group has created a soluble sodium borate glass composition doped with varying amounts of Cerium(IV) Oxide and melted to extract Cerium Oxide nanoparticles with different ratios of  $\text{Ce}^{3+}/\text{Ce}^{4+}$ . We have conducted FTIR study of the parent borate glass, glass doped with Cerium(IV) Oxide, and extracted nanoceria obtained using different extraction mechanisms. Results show direct evidence of O-Ce-O and Ce-O-Ce stretching vibrational bonds in the extracted nanoceria compared to the glass embedded with nanoceria. The Ce-O-B stretching vibration that was visible in FTIR spectra for the nanoceria embedded glass was not found in the extracted nanoceria.

**(GOMD-S1-SP012-2022) Characterization of sodium and calcium addition on aqueous interactions of binary borate glasses by vapor sorption**T. Yin\*<sup>1</sup>; W. C. Lepry<sup>1</sup>; M. T. Islam<sup>2</sup>; I. Ahmed<sup>2</sup>; P. Ouzilleau<sup>1</sup>; K. E. Waters<sup>1</sup>; S. N. Nazhat<sup>1</sup>

1. McGill University, Mining and Materials Engineering, Canada
2. University of Nottingham, Advanced Materials Research Group, United Kingdom

Mineralization of bioactive borate glasses (BGs) in physiological solutions is initiated by ionic exchange and network dissolution of BGs with water. Therefore, understanding these immediate aqueous interactions of BGs is crucial for tailoring them to a desired bioactivity for specific biomedical applications. This study describes a novel technique based on dynamic vapor sorption (DVS) with in-situ Raman spectroscopy to investigate the reactivity and mechanisms of aqueous interactions of BGs. Two melt-quench binary-BGs,  $70\text{B}_2\text{O}_3$ - $30\text{Na}_2\text{O}$  and  $70\text{B}_2\text{O}_3$ - $30\text{CaO}$  (mol%), were investigated to compare the effect of sodium and calcium additions on boron coordination, glass transition temperature, and aqueous interactions, via DVS as well as dissolution in deionized water. DVS, which gravimetrically measures BGs exposed to controlled relative humidity, was applied to evaluate their glass-water reactivity. Meanwhile, in-situ Raman monitored real-time structural changes of two BGs to enlighten their different aqueous reactions. Moreover, correlation of structural changes and reaction rates between vapor- and water-induced reactions validates DVS to evaluate the reactivity of BGs. We believe DVS-in situ Raman provides a more rapid and accurate approach to characterize aqueous reactivity and mechanisms of BGs compared to traditional methods, such as submersion in aqueous solutions.

**(GOMD-S1-P013-2022) Incorporation of  $\text{P}_2\text{O}_5$ ,  $\text{MoO}_3$  and  $\text{ZrO}_2$ -rich dismantling nuclear waste in an alkali-rich glass belonging to the  $\text{SiO}_2$ - $\text{B}_2\text{O}_3$ - $\text{Al}_2\text{O}_3$ - $\text{Fe}_2\text{O}_3$ - $\text{Na}_2\text{O}$ - $\text{Li}_2\text{O}$ - $\text{CaO}$  system**S. Achigar<sup>1</sup>; D. Caurant\*<sup>1</sup>; E. Régnier<sup>2</sup>; O. Majérus<sup>1</sup>; T. Charpentier<sup>3</sup>

1. Chimie Paristech CNRS, institut de recherche de Chimie Paris, France
2. CEA Marcoule, DEN, DE2D/SEVT/LDMC-Marcoule, France
3. NIMBE, CEA, CNRS, University Paris-Saclay, France

Dismantling nuclear facilities leads to radioactive waste which may have highly variable compositions. We focused on the waste coming from the dismantling operation of the reprocessing facility UPI (France), that mainly contains Zr, Si, P, Mo, Fe, Na and Al, and whose activity is mainly due to radioactive  $^{137}\text{Cs}$ . We studied

the ability of an alkali-rich (33 mol% alkali oxides) glass matrix to solubilize  $P_2O_5$ ,  $MoO_3$ ,  $ZrO_2$  and  $Cs_2O$  by melting at  $1100^\circ C$ . To determine its capacity to accept a wide range of waste composition, glass series were prepared and characterized by increasing the total amount of oxides representing the waste (10-30 wt% waste loading) and by varying the relative proportions of  $P_2O_5$ ,  $MoO_3$  and  $ZrO_2$ . It is shown that this matrix accepts a wide range of waste compositions without exhibiting heterogeneities and melt remained homogeneous, but during cooling,  $P_2O_5$  and  $MoO_3$  may lead to phase separation and crystallization ( $Na_2MoO_4$ ,  $CsLiMoO_4$ ,  $NaCaPO_4$ ,  $NaLi_2PO_4$ ,  $Li_3PO_4$ ).  $ZrO_2$  never lead to phase separation or crystallization, possibly because of the existence of strong connections between Zr and Si through Zr-O-Si bonds, whereas P and Mo would be present as  $PO_4^{3-}$  and  $MoO_4^{2-}$  mobile entities non-connected to the silicate network (Raman and  $^{31}P$  MAS NMR studies of simplified glasses). The increasing order of oxides solubility is  $MoO_3 < P_2O_5 < ZrO_2$ . A 10 wt% waste loading appears acceptable as almost all the glass compositions resulting from this loading value were homogeneous after cooling.

### (GOMD-S1-SP014-2022) Correlating Non-Synchrotron X-ray Techniques for Multiscale Imaging of Mo-containing Glasses

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Nuclear waste glasses often contain many complex phase separations and crystals, and understanding these components is key to predicting and engineering glass durability. Large field-of-view X-ray Transmission Imaging, X-ray micro-Computed Tomography ( $\mu CT$ ), X-ray nano-Computed Tomography (nano-CT), Wide Angle X-ray Scattering (WAXS), and Small Angle X-ray Scattering (SAXS) were leveraged to examine molybdenum-containing simulated nuclear waste glasses. Crystal and phase separation features were imaged from 10 nm to 1 mm. For instance, this unique scheme enabled exploration of 5 or more levels of hierarchical glassy phase separation, partitioning of linear dendritic powellite ( $CaMoO_4$ ), and single crystal zircon ( $ZrSiO_4$ ). From the nanoscale to mesoscale, a variety of qualitative and quantitative phase information (such as size, morphology, distribution, and interactions) was elucidated. Reflected-light microscopy, Scanning Electron Microscopy (SEM), Wavelength Dispersive Spectroscopy (WDS), and X-ray Diffraction (XRD) were utilized to verify the results. Combining these techniques can potentially help visualize and evaluate the phases key to long-term durability of vitrified waste, as well as elucidate kinetic processes in complex glasses.

### (GOMD-S1-SP015-2022) Lithium-Iron Silicates as Simulations of High-Fe Nuclear Waste Glass

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The underlying crystallization complexities and resulting properties of simulated nuclear waste glasses provide critical insight to the performance of glass for long-term nuclear waste storage. Specifically, the effect of additional  $Fe_2O_3$  on crystallization may be an important consideration in vitrification of certain wastes. Previous research has shown that compositions simultaneously high in Li and Fe tend to crystallize oxide phases containing both these metals, which are also potentially interesting as low-cost alternative cathodes for batteries. A standard melt-quench technique was implemented to synthesize glasses with compositions  $LiFeSiO_4$ ,  $LiFeSi_2O_6$ , and  $LiFeSi_3O_8$ , which are also Li analogues to natural mineral compositions. X-ray Diffractometry (XRD), Differential Thermal Analysis (DTA), and Vibrating Sample Magnetometry (VSM), were used to observe crystallization behavior. A lithium iron oxide phase

was detected using XRD for all samples melted at  $1300^\circ C$  but was most prominent in the  $LiFeSiO_4$  sample. The thermal measurements revealed crystallization and an increase in glass transition temperature as the silicon to iron ratio increased. VSM data presented a coercivity which was similar to that of magnetite. By correlating the crystal structure of the observed crystalline phase to the DTA and VSM data, new insight regarding the crystallization of alkali-iron compositions with added  $Fe_2O_3$  was obtained.

### (GOMD-S1-P016-2022) Impacts of Cr(III) and Cr(VI) concentrations on key high-level waste glass properties

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This study investigates the effects of chromium concentration and redox on simulated high-level waste (HLW) glass properties in high-chromium Hanford wastes. Thirty glasses with  $1 \leq Cr_2O_3 \leq 2.5$  wt% were fabricated and analyzed. The chemical compositions and Cr redox ratios were measured along with properties of interest to Hanford HLW vitrification: crystal formation after centerline canister cooling (CCC), crystallinity as a function of temperature, viscosity, electrical conductivity, toxic leaching characteristics, product consistency using the product consistency test (PCT), and  $SO_3$  solubility. Only Cr(III) and Cr(VI) were identified in the test glasses and their ratio was found to be largely correlated to optical basicity. For most of the properties, except for PCT, Cr redox appeared to have a significant impact on the property. Most properties were affected differently by Cr(III) than Cr(VI). These affects were quantified and rationalized based on previously studied bonding nature of the two primary oxidation states.

### (GOMD-S1-SP017-2022) Impact of $[Na_2O]/[Al_2O_3]$ ratio and $La_2O_3$ addition on the solubility of molybdenum oxide in aluminoborosilicate glasses

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Molybdenum oxide ( $MoO_3$ ), an integral component of the HLW, exhibits low solubility in peralkaline aluminoborosilicate-based nuclear waste glasses, which limits the overall waste loading capacity of the final waste form. Hence, there is considerable interest in developing new aluminoborosilicate-based glass matrices with an ability to incorporate higher concentration of  $MoO_3$  in their structure. Herein, we report a systematic study conducted to investigate the solubility of  $MoO_3$  in a series of sodium aluminoborosilicate glasses synthesized by varying the  $[Na_2O]/[Al_2O_3]$  ratio (0.8, 1, and 2.5), and further adding 5 mol%  $La_2O_3$ . While preliminary results reveal that the solubility of  $MoO_3$  scales positively with decreasing  $Na_2O/Al_2O_3$  in both  $La_2O_3$ -free and  $La_2O_3$ -containing glasses, no clear impact of  $La_2O_3$  addition on  $MoO_3$  solubility can be established.  $La_2O_3$  improves the solubility of  $MoO_3$  in peralkaline ( $[Na_2O]/[Al_2O_3] = 2.5$ ) glasses, whereas the opposite effect is observed in peraluminous glasses ( $[Na_2O]/[Al_2O_3] = 0.8$ ). This poster will discuss the observed trends in  $MoO_3$  solubility in alkali aluminoborosilicate glasses based on the detailed structural characterization performed on the as-synthesized glasses and glass-ceramics by XRD, SEM-EDS, Raman, and NMR spectroscopy.

### (GOMD-S1-SP018-2022) Preliminary Sintering Study for ZnO-Bi<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub> Binder Glass

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A candidate for a low-temperature glass binder was down-selected after a series of trials, and detailed crystallization studies on this glass were undertaken. The design criteria included a low glass transition temperature ( $T_g$ ) and a large sintering window,  $\Delta T$ , (range between

transition temperature and onset of crystallization), which allows for delayed crystallization due to prolonged viscous flow. From a combined suite of ten (10) explored glasses in the zinc-bismuth-borate and zinc-bismuth-silicate systems,  $25\text{ZnO}-15\text{Bi}_2\text{O}_3-60\text{B}_2\text{O}_3$  ( $\Delta T = 186$ ,  $T_g = 513^\circ\text{C}$ ) was selected, quenched as amorphous glass (as determined by X-ray diffraction), then was further investigated via thermal sintering of pressed powder pellets, heat treated at varying temperatures for 1-4 h. Observed crystalline phases were a zinc tetraborate phase ( $\alpha\text{-ZnB}_4\text{O}_7$ ), observed at short heating times, and a bismuth borate phase ( $\text{Bi}_3\text{B}_5\text{O}_{12}$ ) forming after extended heating (4 h) at  $600^\circ\text{C}$  and  $650^\circ\text{C}$ . Density loss (due to air entrapment) and negative linear shrinkage (due to surface crystallization) were also evident after heating at  $600^\circ\text{C}$  and  $650^\circ\text{C}$ . Further optimization protocols are considered for consolidation of such binder glass, as the ultimate intent is to fuse aluminosilicates containing waste ions, to ensure safe encapsulation of volatile I-129 upon sintering.

#### (GOMD-S1-SP019-2022) Scratch-induced Damage of Graphene-coated Silica Glass: A Molecular Dynamics Study

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Glass surfaces are highly prone to scratch-induced damages during their service life which severely affects the bulk mechanical strength of the glass. Such scratch damages primarily depend on the friction between the glass and rigid counter surfaces. A possible approach for minimizing such friction-induced deformations in glasses is to deposit thin lubricious coatings that are compatible with the glass substrate. To this extent, we study the scratch damage of graphene-coated silica glass against a spherical diamond indenter with Molecular Dynamics (MD) method. The results show a marked reduction in the frictional forces during scratching of the graphene-coated silica glass, as compared to the bare glass surface, thereby implying reduced severity of sliding. The coordination number analysis of the silica glass substrate reveals a considerable reduction in the damage layer thickness beneath the sliding indenter under different applied loads in the presence of graphene coating. Additionally, the stress per atom and Voronoi volume is computed, and their evolution along the scratch trajectory is recorded. The structure of the residual scratched glass is further probed to evaluate the bond angle, intermediate ring, and defect distributions and correlated with the deformation mechanisms. The results provide new insights into the scratch damage of glasses with protective 2-D graphene coatings.

#### (GOMD-S1-SP020-2022) Laser-assisted processing of hermetic glass-to-metal seals

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Glass-to-metal seals are used in a wide range of devices where hermeticity is required to ensure functionality. Typical seals are made by heating components to temperatures high enough to flow the glass and to bond to metals. These processes often limit designs for hermetically sealed components. This paper describes the use of a Nd:YAG laser to directly form hermetic seals in simple geometries with several combinations of glass and metals, including simple pin seals made from stainless steel shells or titanium shells and alloy-52 pins. The glasses were doped with transition metal oxides to vary the bulk absorbance at 1070 nm, but the increase in absorbance with temperature also affected seal quality, including the distance from the sealing surface for bonded glass-metal interfaces.

#### (GOMD-S1-SP021-2022) Effect of Glass Composition on the Laser-Induced Nucleation and Growth of Lithium Niobate Crystals in Lithium Niobosilicate Glass

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The formation of lithium niobate ( $\text{LiNbO}_3$ ) crystals in lithium niobosilicate (LNS) glass via laser irradiation has drawn much attention due to potential device applications based on lithium niobate's favorable optical and electro-optic properties.  $\text{LiNbO}_3$  crystals of different size and morphology, such as nanocrystals and segmented crystal lines, have been fabricated depending on the laser processing parameters employed. In practice, it is challenging to achieve continuous, single-crystal growth of  $\text{LiNbO}_3$  within LNS glass. This work reports on progress in overcoming this challenge by exploring how the formation of single crystal  $\text{LiNbO}_3$  is affected by the incongruent composition of the glass matrix. Measurements of incubation time for the detection of crystal via static irradiation suggest that the glass composition strongly affects the nucleation rate. Through a systematic variation of glass composition ( $(100-x)\text{LiNbO}_3 - x\text{SiO}_2$  for  $x = 22, 26, 30,$  and  $34$ ), laser scanning speed, and laser power, the formation of various crystal morphologies, including cm-long single crystal  $\text{LiNbO}_3$  in certain compositions, is demonstrated. The dependence of crystal morphology on these parameters is explained as an interplay between nucleation and growth, as controlled by the laser scanning speed.

#### (GOMD-S1-SP022-2022) Photo-bleaching of Photo-Thermal-Refractive Glass

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Photo-thermo-refractive (PTR) glass is a recording medium for high-power throughput volume Bragg gratings (VBGs). A byproduct of hologram recording in this glass is additional absorption in visible and near IR spectral regions due to Ag nanocluster accumulation during the development process. It is known that high-power green light decreases this absorption. Samples of PTR glass are recorded and developed and are then irradiated via the focused output of an optical parametric oscillator (OPO) in 50 nm increments from 450 to 650nm with power densities of  $\sim 300\text{MW}/\text{cm}^2$  and dosages of  $\sim 425\text{J}/\text{cm}^2$ . Absorption spectra before and after high-power exposure show that shorter wavelengths reduced absorption throughout the visible spectral region to a greater degree than that of longer wavelengths. The mechanism of the wavelength dependence of photo-bleaching is discussed.

#### (GOMD-S1-SP023-2022) Mixed oxy-sulfide glassy solid electrolyte material: Structural characterization of $0.58\text{Li}_2\text{S} + 0.42[(1-y)\text{SiS}_2 + y\text{LiPO}_3]$

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Mixed oxy-sulfide (MOS) glassy solid electrolytes have proven to be strong contenders for use in solid-state batteries because of their high ionic conductivity and electrochemical stability. The MOS series  $0.58\text{Li}_2\text{S} + 0.42[(1-y)\text{SiS}_2 + y\text{LiPO}_3]$  ( $y = 0.0 - 1.0$ ) was prepared via a melt quench-synthesis. Differential scanning calorimetry (DSC) was used to determine the glass transition and crystallization temperature of these glasses. Fourier transform infrared (FTIR) and Raman spectroscopy were employed to identify the structure in these glasses. Phosphorous will preferentially



associate with sulfur and silicon with oxygen. As such as the  $\text{LiPO}_3$  content is increased, the observed spectra noticeably shift to show case more of these phosphorous-sulfur bonds.

### **(GOMD-S1-SP024-2022) An Investigation of Haven's Ratio in Alkali Silicate Glasses Using Molecular Dynamics**

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Ionic conductivity depends on the diffusion of ions through the glass matrix. The diffusion coefficient ( $D$ ), as defined by Fick, is an easy way to measure this diffusion. Molecular dynamics (MD) allows for the direct measurement of the mean squared displacement (MSD) of diffusing cations, which can be used to calculate  $D$ . One way to compare different diffusion mechanisms is to measure Haven's Ratio ( $H_R$ ), given by the ratio of tracer diffusion coefficient ( $D_T$ ) of ions to the diffusion coefficient from steady-state ionic conductivity ( $D_\sigma$ ) calculated by the Nernst-Einstein equation. A value of  $H_R=1$  indicates that the mechanism of diffusion is the same for ionic conduction as during tracer diffusion. However, a value of  $H_R<1$  indicates that the introduction of an external electric field introduces new possible mechanisms of ionic diffusion. Using MD, the authors have calculated the MSD of three alkali ions (Li, Na, K) at different temperatures in  $\text{SiO}_2$  glass, with and without the influence of an electric field. From this, they calculated  $H_R$  at temperatures from 700K to 1200K. Results found for  $H_R$  generally fall between 0.5 and 1.0, implying that the electric field does introduce new mechanism(s) for ionic diffusion.

### **(GOMD-S1-SP025-2022) Utilizing Electrical Impedance Spectroscopy (E.I.S.) to Observe In-Situ Phase Changes In Lithium Diborate Glass Undergoing Thermal Relaxation**

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Electrochemical impedance spectroscopy (E.I.S.) is a powerful tool for analyzing the electrical and ionic properties of solid state ceramics and glasses as a function of frequency. In this work, E.I.S. was used to monitor the changes in ionic conductivity during the thermal relaxation of lithium diborate glass. Since the conductivity of a material ( $\sigma$  in  $\text{S cm}^{-1}$ ) is proportional to the phase's geometric factor and inversely proportional to the sample's resistance ( $1/R$  l/A), it becomes possible to measure the relative volume of each phase present within the sample. By repeating these tests at a regular interval while a sample is held at a high temperature below the glass transition temperature, the process of relaxation can be observed in real time. E.I.S. measurements were conducted using a Gamry 1010-E potentiostat connected to a custom sample interface mounted inside a furnace. Glass samples were initially made by melting appropriate amounts of  $\text{Li}_2\text{CO}_3$  and  $\text{H}_3\text{BO}_3$ . Crystallization temperatures were obtained by Simultaneous Thermal Analysis (STA). Preliminary results indicate that relaxation can be induced with this methodology, as demonstrated previously in the literature.

### **(GOMD-S1-SP026-2022) Electrochemical characterization of a drawn thin-film glassy mixed oxy-sulfide-nitride phosphate electrolyte material for applications in solid-state batteries**

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Mary Okkema, Madison Olson, Steve W. Martin Thin-film glassy solid-state electrolytes are often considered for applications in energy storage devices; fully-dense thin-film glassy electrolyte materials are able to minimize power loss while suppressing dendrite growth. The glass with the composition  $\text{Na}_4\text{P}_2\text{S}_{5.8}\text{O}_{0.92}\text{N}_{0.18}$  (NaPSON) was chosen because it balances the high conductivity of a sulfide chemistry with the high processability and electrochemical stability of an oxy-nitride chemistry. NaPSON thin-film glassy solid-state electrolyte ribbons with thicknesses that range from 75 to 600  $\mu\text{m}$  were drawn using a process of softening and drawing of a cast and annealed preform. Electrochemical impedance spectroscopy (EIS)

was used on varying thicknesses of thin-film to investigate and compare the ionic conductivity of  $\text{Na}^+$  in the thin film compared to the bulk sample. Area specific resistance models as a function of time were created to compare the trend of bulk and interfacial resistances of different thicknesses. Thin-film samples were made into symmetric cells and cycled. The cycling of the symmetric cells gave insight into the behavior and durability of the electrolyte under applied voltage and sustained current. These results show that drawn thin-film electrolytes are a solid research direction.

### **(GOMD-S1-SP027-2022) Lithium oxysilicate dopants in $\text{Li}_2\text{S} + \text{SiS}_2$ glassy solid-state electrolyte systems**

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The favorable electrochemical properties of glassy solid-state electrolytes based on the  $\text{Li}_2\text{S} + \text{SiS}_2$  series warrant further exploration into the effects of various dopants. The  $\text{Li}_2\text{S} + \text{SiS}_2$  series was modified through doping of lithium oxysilicates at near-eutectic compositions. Precursor oxysilicates were synthesized through high temperature solid-state synthesis of pressed pellets of lithium metasilicate, lithium carbonate, and silica sand. Glassy samples in this series were synthesized via melt quenching of mechanically milled powders. Initial glass transition and crystallization temperatures measured through differential scanning calorimetry (DSC) indicate potentially favorable characteristics for thin-film drawing of the glassy samples. Further DSC cycling experiments were conducted on the glass series to better determine the fragility and viscosity of the series utilizing the Mauro-Yue-Ellison-Gupta-Allan (MYEGA) model. Electrochemical impedance spectroscopy was used to determine temperature-dependent ionic conductivities of the series.

### **(GOMD-S1-SP028-2022) Effect of crystallization on the electrical conductivity of vanado-tellurite glass doped with $\text{CuO}$ , $\text{Cu}_2\text{O}$ , $\text{FeO}$ and $\text{Fe}_2\text{O}_3$**

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Glasses containing transition metal oxides (TMO) are systems of interest due to optical and electrical properties that make them suitable for many uses, including solid-state devices and detectors for physical or medical applications. Among them, vanado-tellurite glasses are well-known for their semiconductor behavior. In this work, four compositions of vanado-tellurite glass doped with  $\text{CuO}$ ,  $\text{Cu}_2\text{O}$ ,  $\text{FeO}$ ,  $\text{Fe}_2\text{O}_3$  were studied to further enhance their electronic conductivity. Samples were prepared by melt-quenching and subsequent thermal treatment to promote crystallization. DC conductivity measurements were performed on both amorphous and crystalline samples, and the electrical properties were measured through impedance spectroscopy and high resistance electrometry. To investigate the influence of the presence and nature of crystalline phase, the samples were investigated by XRD, FEG-SEM-EDS, Raman, FTIR, and density and thermal properties ( $T_g$  and  $\Delta T$ ) were also compared. In general, it was observed that the best conductivity results were obtained for short annealing processes, where morphologically and compositionally homogeneous microstructures were obtained. The best conductivity results were mainly obtained for short annealing processes, where morphologically and compositionally homogeneous microstructures were developed.

### **(GOMD-S1-SP029-2022) Development of cathode materials for use with thin-film glassy solid electrolytes in solid-state batteries**

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The electrochemical and mechanical properties of thin-film glassy solid electrolytes (GSE) in the  $[\text{Li}_2\text{S} - \text{SiS}_2 - \text{LiPO}_3]$  system make them viable candidates for inclusion in solid-state batteries. To properly assess these electrolytes in the full-cell format, compatible composite



cathode materials must be developed. These materials must be electronically and ionically conductive, and form a stable interface in contact with the GSE. A composite blend of lithium iron phosphate ( $\text{LiFePO}_4$ ), a mixed-oxy-sulfide glassy electrolyte, carbon nanotubes, a lithium solvate ionic liquid (SIL), and styrene butadiene rubber binder (SBR) was utilized to create the cathode material. A slurry-casting method was employed to deposit the composite cathode onto the surface of different GSEs: an  $\text{LiPO}_3$  thin-film and a mixed-oxy-sulfide system. Full cells were assembled and assessed using a variety of electrochemical tests. Galvanostatic cycling and cyclic voltammetry exhibit stable cycling behavior, indicating that these slurry-cast cathode materials are viable for usage in solid-state batteries.

#### **(GOMD-S1-P030-2022) Optimization of Antireflective Layers of Silicon Solar Cells: Comparative studies of the Efficiency between Single and Double Layer at the reference wavelength**

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The deposition of an antireflection coating (ARC) on the front side of the solar cells allows a significant reduction of the losses by reflection. It thus allow an increase in efficiency of the cell. Various materials are used as an antireflection layer. For our studies, we focused on the deposition of some materials as an antireflection layer on the solar cell such as  $\text{SiO}_2$ ,  $\text{Si}_3\text{N}_4$ ,  $\text{TiO}_2$ ,  $\text{Al}_2\text{O}_3$ ,  $\text{MgF}_2$ , and studied the efficiency of the latter. A theoretical study of antireflection layers has shown that a single antireflection layer does not have as low a reflectivity as a double antireflection layer over a large wavelength range. Thus, our interest was focused on double and multiple antireflection layers. The influence of parameters such as the thickness of the layer (s) as well as the associated refractive indexes on the optical properties of the antireflective structure has been studied. It was found that there are optimal thicknesses and refractive indices for which the reflectivity of the antireflective system is almost zero over a wider or shorter range of wavelengths. The same phenomena are noted in the study of the external quantum efficiency of the solar cell with these materials. Keywords: Silicon, Antireflective Coatings, Solar Cell.

#### **(GOMD-S1-SP031-2022) Materials Mitigation of Optical Nonlinearities for High Power Fiber Lasers**

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This research studies and advances our understanding of the material science associated with power-scaling in high power fiber-based lasers otherwise limited by optical nonlinearities and thermal management issues. While most fibers being designed for HEL applications are based on large mode area designs, this research continues the approach of focusing on the materials from which the optical fibers are made. Parasitic nonlinear effects such as Transverse Mode Instability (TMI) and stimulated Brillouin or Raman scattering (SBS or SRS, respectively) fundamentally arise from light-matter interactions. Optical fiber compositions can be specifically designed to mitigate not only one given parasitic nonlinearity but can, in some cases, greatly reduce multiple nonlinearities concurrently. Additionally, fiber composition can be designed to reduce heat generation or coupled thermo-optic effects in fiber laser systems. This research leverages industry-standard chemical vapor deposition techniques to improve relevance of findings to commercial laser development and to study intrinsic effects which may otherwise be obscured by extrinsic factors. Examples to be further discussed are fiber designs which leverage differential properties between fiber core and cladding to passively alter their modality through thermo-optic effects.

#### **(GOMD-S1-SP032-2022) Yb-Doped Nanoparticle Silica Fibers for Anti-Stokes Fluorescence Cooling**

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Optical fiber technologies are important in modern life. Active optical fibers doped with rare earth (RE) ions are used to make fiber lasers, which are crucial to many advanced manufacturing and defense applications. However, the heat generated by these devices, especially with the ever-increasing demand for output power, is an issue that must be mitigated by cooling systems that consume extra power and add system complexity. A simpler solution is to design active optical fibers that heat less, or even cool, during operation. This research aims to use Yb-doped alkaline earth (AE; Ca, Sr, Ba) fluoride nanoparticles (NP) in the core of a silica glass optical fiber to control the local glass chemistry around the Yb and reduce the heat generated during operation. High-purity optical fibers were made using a modified chemical vapor deposition (MCVD) process with a non-standard NP suspension doping process that resulted in low-loss fibers comparable to commercial laser fibers. NP-doped fibers were fabricated that exhibited laser cooling through anti-Stokes' fluorescence. Use of these NPs, or in combination with other active RE-doped NPs, allows for the design of simpler fiber laser systems with higher output power.

#### **(GOMD-S1-P033-2022) Novel Low Nonlinearity Optical Fibers Based on the Molten Core Method**

M. Stone\*<sup>1</sup>; A. Vonderhaar<sup>2</sup>; M. Cavillon<sup>3</sup>; T. Hawkins<sup>1</sup>; P. Dragic<sup>2</sup>; J. Ballato<sup>1</sup>

1. Clemson University, Materials Science and Engineering, USA  
2. University of Illinois at Urbana-Champaign, Materials Science and Engineering, USA  
3. University of Paris-Saclay, France

One impediment of the continued advancement of optical fibers for high power applications are optical nonlinearities such as Stimulated Brillouin and Raman Scattering. The power threshold above which these parasitic phenomena occur is proportional to the area of the fiber through which the light travels divided by the gain coefficient of the fiber's material. The conventional approach to mitigating these nonlinearities focuses on making the effective area bigger, but this leads to more complex fiber cores, lower yield in fiber production, as well as other unintended consequences. This research focuses on manipulating the gain coefficient by changing the composition of the fiber core using the molten core method (MCM) for fiber fabrication. This allows for a much more straightforward fabrication process where the material does the work for you, resulting in a much simpler and conventional core/clad fiber design. Using the MCM allows for previously unattainable all-glass fiber core compositions, which can open the doors to many novel fibers with useful optical properties. This paper provides an overview of results to date and offers new insights into future opportunities, glass systems, and properties critical to next-generation fibers.

#### **(GOMD-S1-SP034-2022) North American Summer School on Photonic Materials (NASSPM): Student retrospectives towards their graduate education and future careers**

E. J. Musterman\*<sup>1</sup>; C. Barker<sup>2</sup>

1. Lehigh University, Materials Science and Engineering, USA  
2. Lehigh University, Physics, USA

For over a decade, the international glass community has supported weeklong international schools to teach glass science and engineering to graduate students and postdocs. In addition to these previous schools, the NASSPM at Université Laval focused specifically on optical and photonic materials with the addition of hands-on

laboratory experience. Over 80 students from 12 countries attended this school at various stages of their graduate and post-graduate education. This poster presentation covers student retrospectives on this school nearly three years afterwards. Specifically, we discuss the impact of early introduction to photonics and optics principles and experiences. This includes practice characterizing micro-ring resonators, diffraction grating couplers and liquid crystal displays. Although not always directly applicable to students' graduate research, the school offered a breadth of introductory experiences to students' graduate education. We further explore how the lab experiences supported international and professional connections between the students, academic researchers and industry professionals.

### **(GOMD-S1-P035-2022) Mid-IR absorption in photo-thermo-refractive glass**

P. Shirshnev<sup>\*</sup>; L. Glebov<sup>1</sup>

1. University of Central Florida, CREOL, USA

Absorption spectrum of high purity zinc-alumina-silicate photo-thermo-refractive (PTR) glass within the range 400-1400  $\text{cm}^{-1}$  (25 – 7.14  $\mu\text{m}$ ) is measured. The sample was prepared as a compressed powder tablet that consists from KBr and PTR glass. The spectrum was decomposed to 11 Gaussian bands: 1360  $\text{cm}^{-1}$  (7.35  $\mu\text{m}$ ), 1275  $\text{cm}^{-1}$  (7.84  $\mu\text{m}$ ), 1162  $\text{cm}^{-1}$  (8.6  $\mu\text{m}$ ), 1026  $\text{cm}^{-1}$  (9.74  $\mu\text{m}$ ), 943  $\text{cm}^{-1}$  (10.6  $\mu\text{m}$ ), 890  $\text{cm}^{-1}$  (11.23  $\mu\text{m}$ ), 788  $\text{cm}^{-1}$  (12.69  $\mu\text{m}$ ), 730  $\text{cm}^{-1}$  (13.69  $\mu\text{m}$ ), 660  $\text{cm}^{-1}$  (15.15  $\mu\text{m}$ ), 590  $\text{cm}^{-1}$  (16.94  $\mu\text{m}$ ), 460  $\text{cm}^{-1}$  (21.73  $\mu\text{m}$ ). We assigned a band at 1026  $\text{cm}^{-1}$  as the Si-O-Si asymmetric stretching mode, a band 788  $\text{cm}^{-1}$  as the Si-O-Si symmetric stretching mode, and a band 460  $\text{cm}^{-1}$  as the O-Si-O bending mode. The absorption band at 2060  $\text{cm}^{-1}$  is a second harmonic of 1026  $\text{cm}^{-1}$  mode. The absorption at 3077  $\text{cm}^{-1}$  is a third harmonic of 1026  $\text{cm}^{-1}$  mode. The matrix absorption band at 2532  $\text{cm}^{-1}$  is a combination of the second harmonic of 1026  $\text{cm}^{-1}$  mode with 460  $\text{cm}^{-1}$  mode. The data proposed can be used for further investigations of structural transformations in PTR glass.

### **(GOMD-S1-P036-2022) Modeling the Formation of foam Glass**

T. Keith<sup>\*</sup>; G. Craft<sup>1</sup>; M. Laugen<sup>1</sup>; C. L. Trivelpiece<sup>2</sup>; C. Wilkinson<sup>1</sup>

1. GlassWRX, Department of Research & Development, USA  
2. Savannah River National Lab, USA

Foam glass has recently been touted as an environmental solution as it can be made of recycled materials, has a minimal environmental impact, and has desired properties. These advantages make it of interest for emerging industries however the application is limited as the ability to predict the foaming as a function of glass composition and thermal treatment. In this work, we present a simple method to understand the dynamics of ceramic foam formation based on kinetic modeling as well as a series of new experiments to confirm the models. The ramifications on porous glasses in general are discussed.

**Tuesday, May 24, 2022**

## Award Lectures

### **George W. Morey Award Lecture**

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

**8:10 AM**

### **(GOMD-AW-002-2022) Optical Fiber meets the Periodic Table: The past, present, and future of the molten core method**

J. Ballato<sup>\*</sup>

1. Clemson University, Materials Science and Engineering, USA

Glass, in the form of optical fibers, enables all means of modern communications and a great many other important industrial and consumer uses. However, the principal processes for fabricating optical fiber glasses have the unintended consequences of restricting the range of compositions that can be made into practical fibers. This lecture will discuss the past, present, and future of the molten core method for fabricating a wide variety of novel glassy and crystalline core optical fibers, exhibiting an equally wide variety of fascinating properties not previously known.

## S1: Fundamentals of the Glassy State

### **Structure of Glasses I**

Room: Columbia (Second floor)

Session Chair: Thibault Charpentier, CEA

**9:20 AM**

### **(GOMD-S1-017-2022) Extent of structural disorder in glasses and transparent ceramic from advanced solid-state NMR spectroscopy (Invited)**

F. Fayon<sup>\*</sup>; A. Ridouard<sup>1</sup>; L. Piveteau<sup>1</sup>; C. Genevois<sup>1</sup>; M. Pitcher<sup>1</sup>; M. Allix<sup>1</sup>; D. Massiot<sup>1</sup>

1. CNRS, CEMHTI, France

Transparent inorganic materials, such as glasses, single crystals or transparent polycrystalline ceramics, are developed for many key technological applications such as optical and lighting devices. Although these materials can be designed for similar applications, they generally have very different atomic scale structures and macroscopic properties. In this context, we have recently demonstrated that new transparent massive ceramics consisting of metastable phases can be developed by congruent crystallization of glasses. In this work, we will describe the structural characterization of strontium gallosilicate glasses and a new transparent partially disordered metastable ceramic using state-of-the-art solid state NMR methods at high magnetic field. Using  $^{29}\text{Si}$  through-bond multiple-quantum and  $^{71}\text{Ga}$  very-high-field NMR experiments coupled with DFT calculations, it was possible to characterize and quantify the chemical disorder in the transparent metastable ceramic and in the parent glass. It is shown that although positional and topological ordering occurs in the metastable phase, the Ga/Si chemical disorder remains very close to that in glass. New NMR experiments allowing probing longer range interatomic proximities will be described. The obtained results suggest non-random distributions of Si(OGa) $_{4-n}$ (OSi) $_n$  units, both in the crystalline metastable phase and the glass.

9:50 AM

**(GOMD-S1-018-2022) Effect of adding Al<sub>2</sub>O<sub>3</sub> on the structure and properties of LaB<sub>3</sub>O<sub>6</sub> glass**D. Caurant<sup>\*1</sup>; E. Chesneau<sup>2</sup>; T. Charpentier<sup>3</sup>; O. Majerus<sup>1</sup>

1. Chimie Paristech CNRS, institut de recherche de Chimie Paris, France
2. CNRS, CEMTHI UPR 3079, France
3. NIMBE CEA Paris-Saclay, CEA CNRS Université Paris-Saclay, France

In this work, we studied the effect on glass structure and properties of adding Al<sub>2</sub>O<sub>3</sub> to the LaB<sub>3</sub>O<sub>6</sub> glass ((1-x)LaB<sub>3</sub>O<sub>6</sub>-xAl<sub>2</sub>O<sub>3</sub> with x=0 to 0.44 mol%). The evolution of the borate network and the incorporation of Al<sub>2</sub>O<sub>3</sub> was followed using a multi-spectroscopic approach. The local environment of B, Al and O was followed using MAS and MQMAS NMR (<sup>11</sup>B, <sup>27</sup>Al, <sup>17</sup>O). The global structure of glasses was studied by Raman spectroscopy and the evolution of lanthanide environment was followed by optical spectroscopy (Eu<sup>3+</sup>, Nd<sup>3+</sup>-doped glasses). Whereas the evolution of T<sub>g</sub> exhibits a minimum (x~0.13), the glass stability increases until x~0.35. NMR showed that Al<sub>2</sub>O<sub>3</sub> addition induces a decrease of both BO<sub>4</sub>/BO<sub>3</sub> ratio and NBOs amount. In all glasses, significant amounts of AlO<sub>4</sub>, AlO<sub>5</sub> and AlO<sub>6</sub> units were detected but the proportion of AlO<sub>4</sub> units increases at the expenses of AlO<sub>6</sub> units along the series whereas the proportion of AlO<sub>5</sub> units is constant. NMR and Raman spectroscopies showed the formation of Al-O-B connections at the expense of B-O-B bonds in accordance with the formation during melt cooling or glass heating of LaB<sub>3</sub>O<sub>6</sub> crystals that incorporate Al. Finally, we showed that Eu<sup>3+</sup> ions followed glass structure evolution from an environment consisting of both BO<sub>3</sub> and BO<sub>4</sub> units to an environment with both BO<sub>3</sub> and AlO<sub>x</sub> units.

10:10 AM

**(GOMD-S1-019-2022) Structure and its effect on the crystallization behavior of mold flux glasses in the system CaO-SiO<sub>2</sub>-CaF<sub>2</sub>-B<sub>2</sub>O<sub>3</sub>-Na<sub>2</sub>O: Results from Multinuclear NMR Spectroscopy**T. Yeo<sup>1</sup>; J. Cho<sup>2</sup>; S. Sen<sup>\*1</sup>

1. University of California, Davis, Department of Material Science and Engineering, USA
2. Pohang University of Science and Technology, Graduate Institute of Ferrous & Energy Materials Technology, Republic of Korea

The development of novel mold fluxes has been an active area of investigation to improve the productivity and quality of steel products. These fluxes are multi-component glasses predominantly based on CaO-SiO<sub>2</sub>-CaF<sub>2</sub>; B<sub>2</sub>O<sub>3</sub>, Al<sub>2</sub>O<sub>3</sub> and various alkali oxides are used as additives according to the specific needs of the system. In particular, the addition of alkali oxides results in a “depolymerization” of the silicate network, which contributes to decreasing viscosity and accelerating crystallization kinetics. This study examines the atomistic mechanism of crystallization of cuspidine (3CaO•2SiO<sub>2</sub>•CaF<sub>2</sub>) in CaO-SiO<sub>2</sub>-CaF<sub>2</sub>-B<sub>2</sub>O<sub>3</sub> based melts with the addition of Li<sub>2</sub>O, <sup>7</sup>Li, <sup>23</sup>Na, <sup>19</sup>F and <sup>29</sup>Si magic-angle-spinning, and <sup>7</sup>Li{<sup>19</sup>F} and <sup>23</sup>Na{<sup>19</sup>F} rotational echo double-resonance (REDOR) nuclear magnetic resonance (NMR) spectroscopic results indicate that these glasses are phase separated at the nanoscale with a highly depolymerized phase consisting of Q<sup>0</sup> and Q<sup>1</sup> units and characterized by Ca-F bonds that likely act as the precursor for the crystallization of cuspidine. The role of F on the phase separation in these glasses and the detailed structure and Q-species connectivity in the resulting coexisting phases will be discussed.

10:30 AM

**(GOMD-S1-020-2022) Insight into the partitioning and clustering mechanism of rare earth cations in alkali aluminoborosilicate glasses**H. Kamat<sup>\*1</sup>; F. Wang<sup>1</sup>; K. E. Barnsley<sup>2</sup>; J. V. Hanna<sup>2</sup>; A. Tyryshkin<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers, The State University of New Jersey, Materials Science and Engineering, USA
2. University of Warwick, Department of Physics, United Kingdom
3. Rutgers, The State University of New Jersey, Marine and Coastal Sciences, USA

Rare earth (RE) containing alkali aluminoborosilicate glasses find increasingly broad technological applications, with their further development only impeded by yet-poor understanding of the structure of these glasses. Herein we combine free induction decay (FID)-detected electron paramagnetic resonance (EPR), electron spin echo envelope modulation (ESEEM), and NMR spectroscopies, to examine the local coordination environment and speciation of RE<sup>3+</sup> ions in peralkaline aluminoborosilicate glasses co-doped with Nd<sub>2</sub>O<sub>3</sub> (0.001–0.1 mol%) and 5 mol% La<sub>2</sub>O<sub>3</sub>. Quantitative EPR spectral analysis reveals three distinct Nd<sup>3+</sup> forms coexisting in the glasses: isolated Nd<sup>3+</sup> centers, dipole-coupled Nd clusters, and spin-exchange-coupled Nd clusters, with extensive Nd clustering observed at high [RE<sub>2</sub>O<sub>3</sub>]. ESEEM analysis reveals a Na/Si-rich environment (4 Na per Nd) for isolated Nd<sup>3+</sup> centers and a Na/Si/B-rich environment (2-3 Na and 1-2 B per Nd) for dipole-coupled Nd clusters, while the EPR-silent exchange-coupled RE clusters are predicted to exist in a Na/B-rich environment, thereby suggesting a nanoscale glass-in-glass phase separation induced by the RE<sup>3+</sup> ions. Based on the results, we present a mechanistic model that explains the high tendency of RE<sup>3+</sup> ions to form clusters in alkali aluminoborosilicate glasses.

10:50 AM

**(GOMD-S1-021-2022) Octahedral oxide glass networks at ambient pressure: Structure of neodymium titanate glass**S. K. Wilke<sup>\*1</sup>; O. L. Alderman<sup>4</sup>; C. J. Benmore<sup>2</sup>; J. Neufelnd<sup>3</sup>; R. Weber<sup>1</sup>

1. Materials Development, Inc., USA
2. Argonne National Lab, X-ray Science Division, Advanced Photon Source, USA
3. Oak Ridge National Lab, Neutron Science Division, Spallation Neutron Source, USA
4. Rutherford Appleton Laboratory, ISIS Neutron and Muon Source, United Kingdom

Rare-earth titanates form very fragile liquids that can be made into glasses with high refractive indices (>2.1), low dispersion, and wide transmission range in the visible and infrared spectrum. We investigate the atomic structure of 83TiO<sub>2</sub>-17Nd<sub>2</sub>O<sub>3</sub> glass using X-ray and neutron diffraction with double isotope substitutions for both Ti and Nd. Six total structure factors are analyzed (5 neutron + 1 X-ray) to obtain complementary sensitivities to O and Ti/Nd scattering, and an empirical potential structure refinement (EPSR) provides a structural model consistent with the experimental measurements. Glass density is 4.72(13) g cm<sup>-3</sup>. Mean coordination numbers from EPSR are 5.72(6) for Ti-O and 7.70(26) for Nd-O, in reasonable agreement with neutron first order difference functions for Ti and Nd. The titanate glass network comprises distorted polyhedra of 26% Ti-O<sub>5</sub> and 73% Ti-O<sub>6</sub>, connected via 71% corner-sharing and 23% edge-sharing. The O-Ti coordination environments include 15% nonbridging O-Ti, 51% bridging O-Ti, and 32% tricluster O-Ti. This network of predominantly octahedral-coordinate Ti with significant edge-sharing is highly unusual, especially compared to traditional glass formers like SiO<sub>2</sub>, which comprise corner-sharing Si-O<sub>4</sub> tetrahedra. Additional analyses of the glass structure, including bond angle distributions and ring statistics, are also presented and discussed.



## Topology and Rigidity

Room: Constellation E (Second floor)

Session Chairs: Mathieu Bauchy, University of California, Los Angeles; Morten Smedskjaer, Aalborg University

9:20 AM

### (GOMD-S1-022-2022) Low-Dimensional Representation of the Short- and Medium-Range Structure of Glassy Materials (Invited)

T. J. Hardin<sup>\*1</sup>; M. Wilson<sup>1</sup>; M. Chandross<sup>1</sup>; M. Shields<sup>2</sup>; M. L. Falk<sup>2</sup>

1. Sandia National Laboratories, Computational Materials and Data Science, USA
2. Johns Hopkins University, Materials Science and Engineering, USA
3. Johns Hopkins University, Civil and Systems Engineering, USA

Short- and medium-range order is imposed on glassy materials by the thermodynamic drive towards minimum enthalpy; the atomic configurations comprising a glass can be thought of as being loosely constrained to a manifold which depends on the interatomic energetic specifics of the material. We generated molecular dynamics models of metallic and silicate glasses, compared local atomic environments within each glass using the Gaussian Integral Inner Product distance, and applied hierarchical clustering and diffusion maps to extract low-dimensional discrete and continuous parameterizations of the materials' enthalpic structural manifolds. These structural parameterizations constitute a new, tunably granular, computationally friendly quantification of glassy structure, which is partially interpretable in terms of intuitive physical quantities including aspects of topology in covalent glasses. This presentation will cover both our structure-parameterization methodology and resulting physical insights, and will look forward to mapping from structure to mechanical properties. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525 (SAND2022-0097 A).

9:50 AM

### (GOMD-S1-023-2022) Molecular origin of the super-strong behavior of melt dynamics in the Intermediate Phase of chalcogenide glasses

B. S. Almutairi<sup>\*1</sup>; R. Chbeir<sup>2</sup>; A. Welton<sup>2</sup>; M. Burger<sup>2</sup>; S. Chakravarty<sup>3</sup>; P. Boolchand<sup>2</sup>

1. Princess Nourah Bint Abdulrahman University, Physics, Saudi Arabia
2. University of Cincinnati, Electrical Engineering and Computer Science, USA
3. University of Cincinnati, Mechanical and Materials Engineering, USA

Delayed homogenization of Chalcogenide glasses/melts first emerged when bulk  $\text{Ge}_x\text{Se}_{100-x}$  glasses were synthesized, and their homogeneity tracked periodically in ex-situ FT-Raman profiling. Results showed that even 2 gram sized batches took nearly 7 days to fully homogenize when alloyed at 950°C. Modulated-DSC measurements showed such glasses show a square-well like variation of the Enthalpy of relaxation at  $T_g$ ,  $\Delta H_m$ , defining the Intermediate Phase (IP). Melt fragility index,  $m(x)$ , showed a Gaussian-like global minimum ( $m = 15$ ) near the center of the IP range. Strikingly parallel results have since emerged in several families of Chalcogenides. Here we report results on ternary  $\text{Ge}_x\text{As}_x\text{S}_{100-2x}$  glasses and show that decoupled  $\text{S}_8$  rings and  $\text{As}_4\text{S}_4$  and  $\text{As}_4\text{S}_3$  cages from the 3D backbone also influence the melt fragility index. IP melts are found to be super-strong with  $m = 15$  at  $x = 15\%$ , with presence of decoupled  $\text{S}_8$  rings shifting the global minimum of  $m(x)$  from IP center to upper edge of the IP near the stress transition.

10:10 AM

### (GOMD-S1-024-2022) Structure-property relationship in covalent network glasses: Relative influence of three structural features

P. Lucas<sup>\*1</sup>

1. Univ of Arizona, USA

The search for a simple correlation between structure and properties has long been an overarching goal of glass science. In that respect, chalcogenide glasses have been the subject of extensive studies

due to the well-defined nature of their covalent network which permits accurate determination of bond numbers, bond angles and local geometries such as tetrahedra, trigonal pyramids, chains, etc. Following the observation of a correlation between glass-formation and constraint counting in Ge-Se glasses, topological theories have largely dominated the field of structure-property relationship in chalcogenide glasses. Here we present a systematic analysis of a large body of literature data from independent sources to determine the relative influence of topology, stoichiometry and dimensionality on the trends in density and fragility in the Ge-As-Se, As-Se and Ge-Se systems. It is found that stoichiometry is the largely dominant influence in predicting trends in physical properties, followed by dimensionality. Topological contributions are only observed in the Ge-Se system when contributions from stoichiometry and dimensional effects are absent. However, even in this system, structural heterogeneity can be invoked to explain trends in physical properties.

10:30 AM

### (GOMD-S1-025-2022) Learning topology of disordered materials through graph neural network

N. Krishnan<sup>\*1</sup>; V. Bihani<sup>1</sup>; S. Manchanda<sup>1</sup>; S. Ranu<sup>1</sup>

1. Indian Institute of Technology Delhi, Civil Engineering, India

Glasses are traditionally prepared by cooling a liquid fast-enough to avoid crystallization. Despite the variation in potential energies, glasses obtained at different cooling rates show similar short- and medium-range orders. In this work, we investigate the local structure of such disordered system by utilizing an unsupervised machine learning approach employing graph neural networks. Specifically, we prepare the well-established 2D binary LJ glass structures of composition A65B35 at different cooling rates ranging from  $3.33 \times 10^{-3}$  to  $3.33 \times 10^{-6}$ . Graph based structures where nodes represent atoms are obtained from the simulation trajectories. We train an unsupervised random walk-based graph neural network model to learn node representations capturing local structural properties of the node's neighborhood. To analyze the local structures, we perform clustering of nodes based upon their node representations. Interestingly, we observe that these clusters exhibit notably different potential energy—with low and high energy clusters within the glass structure. In order to analyze the stability of these clusters, the mean squared displacements were computed. We observe a positive correlation between the average potential energy of the clusters and the mean square displacement, suggesting a structure-dynamics correlation in these systems.

10:50 AM

### (GOMD-S1-026-2022) Understanding diffraction patterns and topologies of disordered materials (Invited)

Y. Onodera<sup>\*1</sup>; S. Kohara<sup>2</sup>

1. Kyoto University, Institute for Integrated Radiation and Nuclear Science, Japan
2. National Institute for Materials Science (NIMS), Japan

The structure of glassy, liquid and amorphous materials is still not well understood, due to the insufficient structural information from diffraction data. We attempted to understand the origin of diffraction peaks, particularly of the first sharp diffraction peak (FSDP,  $Q_1$ ), the principal peak (PP,  $Q_2$ ), observed in the measured diffraction patterns of disordered materials. It is confirmed that the FSDP appears as the results of a sparse distribution of planes in polyhedra. It is found that the PP reflects orientational correlation of polyhedra. Moreover, information of the topology of disordered materials was revealed by utilizing persistent homology analyses. The persistence diagram of silica ( $\text{SiO}_2$ ) glass suggests that the shape of rings in the glass is similar not only to those in the crystalline phase with comparable density ( $\alpha$ -cristobalite), but also to rings present in crystalline phases with higher density ( $\alpha$ -quartz and coesite); that is thought to be a signature of good glass-forming ability in  $\text{SiO}_2$  glass.



Furthermore, we succeeded in characterizing the network topology in densified SiO<sub>2</sub> glasses that were synthesized by using hot or cold compression in terms of persistent homology. Our series of analyses demonstrated that a combination of diffraction, computer simulation and topological analyses is a useful tool to uncover structural features hidden in halo pattern of disordered materials.

**11:20 AM**

**(GOMD-S1-027-2022) Glass Irradiation: Impact on Structure and Mechanical Properties**

M. M. Smedskjaer<sup>\*1</sup>; T. Du<sup>1</sup>; X. Ren<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark

Heavy ion irradiation can modify the surface structure of glasses and consequently their mechanical properties. Here, we attempt to clarify structure-property relations in two families of irradiated glasses. First, in calcium aluminoborosilicate glasses, we use a combination of experiments and atomistic simulations and find that the ion irradiation reorganizes the borate subnetwork through a partial transformation of tetrahedral to trigonal boron units and a coarsening in the distribution of loop structures. This leads to an improvement in both the resistance to crack formation and crack growth as irradiation induces coordination defects that act as local reservoirs of plasticity by allowing more bond switching activities. Second, in organic-inorganic hybrid systems, we simulate irradiation of both zeolitic imidazolate framework crystals and glasses. We track the convergence of the two phases toward a new disordered state upon irradiation, with simultaneous evolution of both structure and mechanical properties. Both studies therefore help to establish structure-property relations in forbidden glass states that are not accessible through any thermal path.

**11:40 AM**

**(GOMD-S1-028-2022) A More Suitable Way to Calculate Glass Packing Fraction and its Application for Young's Modulus Prediction (Invited)**

Y. Shi<sup>\*1</sup>; A. Tandia<sup>1</sup>; S. Elliott<sup>2</sup>; M. Bauchy<sup>3</sup>

1. Corning Incorporated, USA

2. University of Oxford, United Kingdom

3. University of California, Los Angeles, USA

Makishima-Mackenzie (MM) model expresses the Young's modulus of glass by two factors, dissociation energy and atomic packing fraction. This model offers a clear physical picture to understand the compositional dependence of glass stiffness, but it generally underestimates the Young's modulus for many glasses. We argue that the inadequacy of the MM model mainly arises from its definition of the atomic packing fraction—which is defined as the ratio between the volumes of the atoms and the actual macroscopic volume of the glass. Such a definition results in a considerable amount of spacing within the basic building units being counted as free volume, which eventually leads to low packing fractions and to low Young's modulus values. Here we propose a more suitable packing metric, the Rigid Unit Packing Fraction, which defines the basic building units as fully-filled, whole polyhedra made of "touching" oxygen atoms with no interstitial free volume. Young's moduli of 155 oxide glasses predicted from our revised MM model show a significantly improved agreement with experimental data as compared to the original MM model. This study not only improves the ability of the physics-based MM model to yield accurate predictions of the Young's modulus, but also supports the relevance of rigid-unit theory, which could be applied as a basis to decipher other property-structure correlations.

**12:10 PM**

**(GOMD-S1-029-2022) Decoding the Topological Origin of the Thermal Expansion of Glasses**

Q. Zhou<sup>1</sup>; M. Bauchy<sup>\*1</sup>

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

When subjected to variations in temperature, silicate glasses exhibit some thermal expansion—which can negatively affect the performance of substrate glasses for display applications. Interestingly, the coefficient of thermal expansion of silicate glasses exhibits a great compositional variability. In particular, glassy silica presents a usually low coefficient of thermal expansion as compared to other oxide glasses. To date, it remains unclear how the propensity for a glass to expand upon heating is encoded in its atomic structure. Here, we investigate the structural origin of thermal expansion by force-enhanced atomic refinement (FEAR) simulations of several silicate glasses [1]. We demonstrate that FEAR yields an improved description of the temperature-dependent structure of silicate glasses as compared to traditional melt-quench molecular dynamics simulations. Based on these results, we show that the thermal expansion of silicate glasses is encoded in their size and shape of their network rings.

**S2: Glass and Interactions with Its Environment: Fundamentals and Applications**

**Dissolution and Interfacial Reactions III: Modeling Glass Dissolution and Glass Interaction with Various Environments**

Room: Constellation C/D (Second floor)

Session Chairs: Joseph Ryan, Pacific Northwest National Lab; Nicholas Stone-Weiss, Corning Incorporated

**9:20 AM**

**(GOMD-S2-025-2022) Advances of atomistic computer simulations in understanding glass-water interactions (Invited)**

T. S. Mahadevan<sup>\*1</sup>; J. Du<sup>1</sup>

1. University of North Texas, Materials Science and Engg, USA

Interactions between water and silicate glasses have been an active area of research in glasses science due to their importance in biomedicine, microelectronics, architecture, display, packaging, as well as in nuclear waste management. While experimental characterizations of the characteristics of this glass-water interface or alteration layer is done by accessing the local nano-scale environment through techniques such as NMR, TEM, nano-SIMS etc., accurate high-fidelity molecular dynamics (MD) simulations, especially those with reactive potentials, are often used as complementary means of gaining information of the local structural evolution and reaction mechanisms. The emergence of reactive forcefields in MD simulations and Monte Carlo simulations based on realistic glass structures have opened up access to understanding reactions and transport phenomena in the alteration layer in greater details. In this presentation, we review some of the recent advances in which molecular dynamics can be used to study glass water interactions, including the reaction and ion-exchange mechanisms, ion transport, and structural evolution in these alteration layers. Some of the interesting findings that have been discovered based on a combination of MD methods and experimental methods will be presented and we will finish with some thoughts of future directions of the field.

9:50 AM

### (GOMD-S2-026-2022) Quantitative Structural Property Relationship analysis of dissolution rate of aluminosilicate and borosilicate glasses

J. Du<sup>\*1</sup>; X. Lu<sup>2</sup>; J. Vienna<sup>2</sup>; J. V. Ryan<sup>2</sup>; M. Bauchy<sup>3</sup>; J. Delaye<sup>4</sup>; S. Gin<sup>4</sup>

1. University of North Texas, Materials Science and Engineering, USA
2. Pacific Northwest National Laboratory, USA
3. UCLA, USA
4. CEA, France

Quantitative structure-property relationship (QSPR) analysis based on molecular dynamics simulations is a valuable approach to find property-composition correlations of glass materials. This is especially so for properties that are too complex to be directly calculated such as dissolution rate and hardness. In this talk, we will show the application of MD based QSPR analysis of the initial dissolution rate of a series borosilicate and aluminosilicate glasses recently measured. Based on the composition dependent potentials developed in our group, the glass structures were simulated and the structural features were used to construct the structural descriptors. The effectiveness of the various descriptors ranging from simple structural information such as network connectivity, percentage of bridging oxygen, to average ring size and more complex descriptors were tested. The results show that combining MD simulations and QSPR analysis a promising tool to evaluation composition property relations and new composition design.

10:10 AM

### (GOMD-S2-027-2022) Predictive Modeling of Stage III Leach Rate Resumption in Nuclear Waste Glasses

I. S. Muller<sup>\*1</sup>; K. Gilbo<sup>1</sup>; I. Pegg<sup>1</sup>

1. The Catholic University of America, Vitreous State Laboratory, USA

A striking feature observed in leaching tests performed on many nuclear waste glasses is the sudden increase in leaching rate after a period (Stage II), which can be very long, during which the rate is low. In the period following this “resumption” (Stage III) the rate can approach that of the initial rate (Stage I). This behavior presents considerable challenges for prediction of long-term performance. Of particular interest is the ability to predict the time at which resumption occurs and whether it occurs. In this paper, we present the results from an analysis of data that we have collected on numerous nuclear waste glasses spanning a wide range of composition subjected to over 30 years of continuous glass leaching. The resumption times also cover a wide range, from 81 to 7832 days. We show that clear glass composition effects on the time to resumption are evident and quantifiable. The data are analyzed using segmented linear regression in combination with mixture models. The results of this analysis, model comparisons and performance, model validation using a separate set of data, and the derived compositional trends will be presented and discussed.

10:30 AM

### (GOMD-S2-028-2022) Dissolution behavior and kinetics of alkali/alkaline-earth aluminoborosilicate glasses in hyperalkaline media: Impact of high ionic field strength non-framework cations

Q. Qin<sup>\*1</sup>; N. Stone-Weiss<sup>1</sup>; T. Zhao<sup>2</sup>; P. Mukherjee<sup>3</sup>; J. Ren<sup>2</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Key Laboratory of Materials for High-Power Laser, China
3. Michigan Technological University, Materials Science and Engineering, USA

Understanding the impact of constituent oxides on glass corrosion behavior and its dependence on surrounding environment has attracted extensive research interest as it plays a key role in designing new glass compositions for industrial application. Nowadays, non-framework high field strength cations, such as Li<sup>+</sup>,

Ca<sup>2+</sup>, and Zr<sup>4+</sup>, are often seen in industrial-relevant glasses including nuclear waste glass, high-strength glass-ceramics and optical glasses. However, their influence on the chemical durability of the resultant glasses is unclear. Therefore, this study aims to gain new insights into the impact of HFSCs on the corrosion of alkali/alkaline-earth aluminoborosilicate glasses. Eleven alkali/alkaline-earth aluminoborosilicate glasses containing different HFSCs (i.e., Li<sup>+</sup>, Ca<sup>2+</sup>, La<sup>3+</sup>, Zr<sup>4+</sup>, Ti<sup>4+</sup>, and Nb<sup>5+</sup>) have been synthesized and their dissolution behavior in TMAH solution at pH = 13 has been investigated. Combining various advanced characterization techniques, we are able to monitor the structural and chemical evolution of the glasses (both in bulk and at surface) as a function of dissolution kinetics and demonstrate the effect of HFSCs on the short- and long-term durability of the glasses in hyperalkaline environment.

10:50 AM

### (GOMD-S2-029-2022) Predicting mineral wool fibers dissolution in biological environments by in vitro tests and thermodynamics

N. Drnovsek<sup>\*1</sup>; U. Kovacic<sup>1</sup>; D. Trivunčević<sup>2</sup>; M. Debeljak<sup>1</sup>; E. Pezennec<sup>1</sup>; P. Kiefer<sup>1</sup>; D. Laurent<sup>1</sup>; J. DeMott<sup>1</sup>; M. Strlič<sup>2</sup>; R. Conrad<sup>3</sup>

1. Knauf Insulation, Slovenia
2. Faculty of Chemistry and Chemical Technology, Slovenia
3. UniglassAC GmbH, Germany

In the European Union, glass and stone mineral wool fibers are classified as a potential carcinogen to humans. Carcinogenicity was proven to be driven by fibers biopersistence in the lungs [1]. Fibers can be exonerated from being classified as carcinogenic, if weighted fiber half-life is less than 10 or 40 days, for inhalation and intratracheal instillation test, respectively [2]. The biopersistence can be measured in vitro by assessing the fibers' ability to dissolve in simulated lung fluids (SLF). Although many SLFs have been used in the published literature, mimicking a complex lung environment is difficult. SLF components can affect the dissolution kinetics of the mineral fibers differently, depending on the solution's ionic strength, pH, and species formation between dissolved ions from mineral fibers and the solution ionic components. Therefore, to predict in vivo behavior, the choice of the solution and the test conditions are important. To understand the role of lung fluid composition and in vitro test conditions, the influence of a wide selection of simulated lung solutions and their components, on the dissolution of glass and stone mineral wool fibers were evaluated and compared in the present study. The experimental data of in vitro tests were supported by a thermodynamic approach, by calculating species formation and possible precipitates.

11:10 AM

### (GOMD-S2-030-2022) Aging Effects on the Failure Characteristics of Ion Exchanged Alkali Aluminosilicate Glass

R. Grodsky<sup>\*1</sup>; R. Brow<sup>2</sup>

1. Honeywell FM&T, USA
2. Missouri University of Science & Technology, Materials Science & Eng, USA

The widespread use of ion exchanged glass in modern devices makes understanding the age-induced degradation mechanisms a key area of study. Flat coupons of alkali aluminosilicate glass were ion exchanged in KNO<sub>3</sub> salt baths and then either: 1) heat treated at 70 °C in an 85% relative humidity environment for one week, or 2) submerged in distilled water at 70 °C for varying lengths of time. Indentation and ring-on-ring testing were performed to characterize the effects of these post-processing conditions on mechanical properties and were supplemented by fractography analyses of samples after fracture. Glass surfaces were characterized by a number of techniques, including x-ray photoelectron, IR and Raman spectroscopies. Changes in surface chemistry were correlated to trends in failure strength and fracture behavior.

11:30 AM

**(GOMD-S2-031-2022) Quantifying residual stress during case II diffusion of water in Na<sub>2</sub>O-3SiO<sub>2</sub> glass**B. D. Hausmann<sup>\*1</sup>; M. Tomozawa<sup>1</sup>

1. Rensselaer Polytechnic Institute, Materials Science &amp; Engineering, USA

Sodium silicate glass has been found to exhibit case II diffusion behavior with water: At low temperatures, the depth of water diffusion progresses linearly with time. This deviation from behavior described by Fick's law may be a result of diffusivity that is significantly affected by water concentration and/or residual stress at the diffusion front. To clarify the role of residual stress in case II diffusion, Na<sub>2</sub>O - 3SiO<sub>2</sub> glass was heat treated at 80°C in a saturated water vapor environment. Residual stress was measured at the interface formed by the diffusion front. It was found that the magnitude of residual stress gradually decreases from 2~48 hours of heat treatment while remaining present throughout. This result indicates that residual stress at the diffusion front is likely a dominant cause of case II diffusion in Na<sub>2</sub>O - 3SiO<sub>2</sub> glass.

**Nuclear Waste Immobilization I**

Room: Frederick (Second floor)

Session Chair: John McCloy, Washington State University

9:20 AM

**(GOMD-S2-032-2022) Effect of melter feed composition and properties on the rate of melting during vitrification of nuclear waste (Invited)**R. Pokorný<sup>\*1</sup>; J. Klouzek<sup>1</sup>; M. Vernerová<sup>1</sup>; P. Ferkl<sup>2</sup>; J. Marcial<sup>2</sup>; S. Lee<sup>2</sup>; P. Hrma<sup>2</sup>; A. A. Kruger<sup>3</sup>

1. University of Chemistry and Technology Prague, Czechia
2. Pacific Northwest National Lab, USA
3. US Department of Energy, Office of River Protection, USA

The rate of conversion of nuclear waste melter feed to glass is affected by the selection of melter feed materials and by melter operating conditions. Recently, we developed a melting rate correlation equation (MRC), which relates the glass production rate with two types of variables: (a) feed and melt properties: conversion heat, cold-cap bottom temperature, and glass melt viscosity; and (b) melter design and operation parameters: melter geometry, melter operating temperature, and gas bubbling rate. The MRC shows good agreement for an extended melting rate data set of high-level waste (HLW) melter feeds and a data set generated for low-activity waste (LAW) melter feeds. Although the MRC can estimate the rate of melting based on the properties (conversion enthalpy, cold cap bottom temperature) of a particular waste feed, and thus qualifies as a promising tool to support the selection of glass forming and modifying additives (GFMA's), there is currently no model or algorithm to quantify the effect of individual GFMA's on these properties and thus optimize the chemical and mineralogical form of feed components and their particle sizes. A feed formulation variation study is currently performed to address this missing link.

9:50 AM

**(GOMD-S2-033-2022) Low Activity Waste Glass Optimization with Machine Learning**X. Lu<sup>\*1</sup>; J. Vienna<sup>1</sup>

1. Pacific Northwest National Lab, Energy and Environment Directorate, USA

The United States Department of Energy is responsible for managing the legacy nuclear waste stored at the Hanford Site. The waste will be vitrified separately as low-activity waste and high-level waste fractions. Waste glass formulation algorithms were developed previously using traditional methods based on property-composition models (e.g., partial quadratic mixture models). Machine learning (ML) has been successfully used to predict glass properties and

discover new glass materials. It is possible to take advantage of the recent developments in ML tools to waste glass formulation. In this proof-of-principle study, ML algorithms such as Gaussian process regression, k-nearest neighbor and artificial neural network were firstly evaluated for use in interpolating glass properties (e.g., viscosity, electrical conductivity, durability). After selecting an appropriate ML data interpretation method, an optimization program was developed to formulate glass compositions to maximize waste loading while simultaneously satisfying property within prediction uncertainties and composition constraints. Results of the waste loadings and glass masses were compared to the ones obtained from using the traditional (mixture model-based) methods. This optimization routine can be easily updated with new glass data and new interpolation methods, opening an efficient pathway to improve nuclear waste glass compositions in the future.

10:10 AM

**(GOMD-S2-034-2022) Understanding the Effects of Anions on Sulfate Retention in Low Active Waste Glasses**N. J. Smith-Gray<sup>\*1</sup>; N. Stone-Weiss<sup>1</sup>; J. M. Lonergan<sup>2</sup>; J. McCloy<sup>1</sup>

1. Washington State University, Materials Science and Engineering, USA
2. Pacific Northwest National Lab, USA

Several challenges arise with the vitrification of low-active nuclear waste (LAW) at Hanford, including salt formation. Production of a molten salt causes detrimental effects to a melter and the vitrification process, as well as the risk of radioactive elements partitioning into non-durable phases. In LAW, the formation of this salt is dominated by the incorporation behavior of sulfur (as sulfate) in the glass. The aim of the present study is to understand the structural effects of various anion additives (e.g., P, Cl, F, Cr) upon a simplified sulfate-containing simulated LAW glass, and therefore how sulfate incorporation in the glass is impacted. To achieve a comprehensive understanding of these systems, various analytical techniques, including pair distribution function analysis, nuclear magnetic resonance, and Raman spectroscopy were utilized to investigate changes in the glass structure. Additionally, X-ray diffraction and electron probe microscopy determined the elemental compositions and crystalline phases within the glasses.

10:30 AM

**(GOMD-S2-035-2022) Effect of iron and chromium on sulfur solubility in alkali borosilicate glasses**X. Xu<sup>\*1</sup>; S. Kamali<sup>2</sup>; A. Pedone<sup>3</sup>; A. Tyryshkin<sup>4</sup>; A. Goel<sup>1</sup>

1. Rutgers University, MSE, USA
2. Tennessee Space Institute, USA
3. University of Modena and Reggio Emilia, Italy
4. Rutgers University, USA

The US-DOE is considering implementing the direct feed approach to expedite the vitrification of radioactive waste stored at the Hanford site. If implemented, the increased sulfate content in direct-feed HLW poses a challenge for the established models for predicting the sulfur solubility in glassy waste forms and is expected to aggravate the complexity of HLW vitrification. Therefore, to design advanced glass formulations with enhanced waste loadings, it is essential to comprehend the fundamental compositional and structural drivers governing the sulfur solubility in borosilicate glasses. Accordingly, the present investigation reports on the impact of Fe<sub>2</sub>O<sub>3</sub> and Cr<sub>2</sub>O<sub>3</sub> on the sulfur solubility in simplified nuclear waste glasses. A combined approach of spectroscopic techniques, including Mossbauer, Raman and ICP-OES spectroscopies, and molecular dynamics simulation are employed to unearth the effect of Fe<sub>2</sub>O<sub>3</sub> on sulfur solubility; and EPR spectroscopy is employed to probe the change in Cr environment during sulfur incorporation.



10:50 AM

### (GOMD-S2-036-2022) Re Volatilization during Nuclear Waste Vitrification: The Salt Effects

C. Niu<sup>1</sup>; L. Peng<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State Key Laboratory of Silicate Materials for Architectures, China

Vitrification is a widely acceptable technology to immobilize nuclear wastes, whereas the high volatility of Tc at elevated temperatures has been the primary concern in vitrifying Tc-bearing nuclear wastes. Several factors, such as inorganic salts including nitrate/nitrite and sulfate, foaming of the feed and REDOX of the melt could co-affect Tc retention in the waste glass, among which inorganic salts are quite crucial to Tc volatilization. Thus, this work investigates the effect of salts including nitrate and sulfate on potassium perchlorate (Re as a non-radioactive surrogate to Tc) volatilization in series of simplified feeds, to clarify the volatilization mechanism of Tc/Re in the presence of salts. The mixtures of  $KReO_4$ ,  $KNO_3/K_2SO_4$  and  $SiO_2$  with varied mass ratios were placed in corundum crucibles, and then heated from room temperature to target temperatures at the heating rate of 5K/min. Thus, obtained samples were analyzed with XRD, XRF, TG-DSC and SEM-EDX. The evolved gas was measured with TG-GC-MS. Finally, the volatile species of  $KReO_4$  and the effects of nitrate and sulfate on  $KReO_4$  volatilization will be discussed.

11:10 AM

### (GOMD-S2-037-2022) Development of Phosphate Glass Waste Forms To Immobilize Salt Waste Stream

M. Tang<sup>1</sup>

1. Clemson University, Department of Materials Science & Engineering, USA

Glass waste forms are currently used to stabilize legacy high-level waste (HLW) materials, and vitrification is the baseline technology for treatment of HLW that would result from reprocessing commercial used nuclear fuel. Due to the low solubilities (< 1.5 mass% for silicate-based glass) of the chloride/fluoride ions and evolution of  $Cl_2/F_2$  gas from the melt under operation temperature, it is not suitable to employ the borosilicate glasses as the host for the full-salt waste streams. Phosphate glass, especially iron phosphate glass, exhibited promising properties as waste form candidates including good chemical durability; high solubility for many heavy metals (e.g., uranium, cesium, molybdenum), noble metals, and rare earths, at intermediate melting temperatures (950 – 1,200 C). In this study, our focus is to develop and optimize highly durable and easily processable iron phosphate glass waste forms to immobilize the salt streams from advanced nuclear fuel cycle by tailoring the composition of the glasses. We also explore low melting temperature (400-500 C) stannous phosphate glass for efficient salt waste form solution. In laboratory test, these phosphate glasses could load up to 50 wt% salt waste streams. The preliminary result shows promising for these phosphate glass waste forms being an improvement over other candidate waste forms.

11:30 AM

### (GOMD-S2-038-2022) Dechlorination and Vitrification of Electrochemical Processing Salt Simulant

Y. Dong<sup>1</sup>; Z. Jia<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State Key Laboratory of Silicate Materials for Architectures (SMART), China

Electrochemical processing of spent fuel in chloride molten salts is a promising option for achieving a closed nuclear fuel cycle, whereas this kind of salt wastes is not applicable to the conventional solidification process due to the low compatibility of chloride ions in glasses. Thus, this work developed a dechlorination-vitrification approach to immobilize chloride salt wastes. The metal chlorides were converted to oxide forms at low temperature and then immobilized in the borosilicate glass. The results show that the dechlorination efficiency could reach more than 99% at 300°C,

when the dechlorination process was optimized. The chlorine in salt wastes was removed in the form of hydrogen chloride, while metal cations were converted to carbonates. The residual metal carbonates were finally vitrified into a borosilicate glass form and the waste loading could be >30 wt%.

11:50 AM

### (GOMD-S2-039-2022) Dependence of Monofrax™ K-3 refractory corrosion on the melt chemistry

X. Xu<sup>1</sup>; R. Saini<sup>2</sup>; K. Akdoğan<sup>1</sup>; A. Goel<sup>1</sup>

1. Rutgers University, MSE, USA

2. Akal University, India

The corrosion of K-3 refractory during the vitrification of nuclear waste is a serious problem, as it affects the performance and lifetime of the melter. Therefore, it is crucial to understand the corrosion behavior of K-3 refractory as a function of glass chemistry. However, the literature on this subject is scarce. In this study, we have focused on unearthing the impact of glass network formers, i.e.  $SiO_2$ ,  $B_2O_3$  and  $Al_2O_3$ , on the corrosion of Monofrax™ K-3 refractory. The corrosion tests have been performed in  $Al_2O_3$  crucibles at 1150°C for 5 days, in accordance with the ASTM C621. The chemical interactions at the melt-refractory interface have been followed using SEM-EDS, XRD, and ICP-OES. According to the elemental diffusion profiles across the glass-refractory interface, a description of the refractory corrosion mechanism is also proposed in this study.

## S4: Glass Technology and Cross-Cutting Topics

### Batch to Glass Conversion

Room: Constellation F (Second floor)

Session Chairs: Jonathan Icenhower, Corning Incorporated;

Irene Peterson, Corning Incorporated

9:20 AM

### (GOMD-S4-014-2022) In-situ visual observations of glass melting processes for nuclear waste vitrification (Invited)

J. Marcial<sup>2</sup>; R. Pokorny<sup>1</sup>; J. Klouzek<sup>1</sup>; M. Vernerova<sup>1</sup>; P. Ferkl<sup>2</sup>; P. Hrma<sup>3</sup>;

A. A. Kruger<sup>4</sup>

1. University of Chemistry and Technology, Prague, Laboratory of Inorganic Materials, Czechia

2. Pacific Northwest National Lab, USA

3. AttainX, USA

4. DOE Office of River Protection, USA

High-temperature visual observation of glass melting has been used for decades to understand the various processes that happen during glass production. Despite its seemingly low-degree of complexity, visual observations are still broadly used today to investigate batch-to-glass conversion, bubble nucleation, fining, or refractory corrosion. For nuclear waste vitrification, visual observations provide a cost-effective method to investigate the influence of waste feed composition and makeup on the conversion process. We will present the overview of our experimental configurations used to study various melting processes, with specific focus on the foaming during batch-to-glass conversion. Two primary techniques include: (i) the so-called feed expansion test (FET) and (ii) a special observation setup under development in which foam is observed during longer timescales of batch conversion to glass along the melting interface through X-ray tomography. Although there are differences in growth and collapse of the foam layer at the bottom of a batch blanket compared to foam observed in a sample during laboratory experiments, these observational techniques still provide insight into the kinetics of the conversion processes by indicating the total amount of foam generated and temperatures of foaming onset and foam collapse.



9:50 AM

**(GOMD-S4-015-2022) Batch-to-glass conversion kinetics in joule-heated melters (Invited)**P. Ferkl<sup>\*1</sup>; P. Hрма<sup>2</sup>; A. Abboud<sup>3</sup>; D. P. Guillen<sup>3</sup>; M. Vernerová<sup>4</sup>; J. Klouzek<sup>4</sup>; J. Marcial<sup>1</sup>; M. Hall<sup>1</sup>; A. A. Kruger<sup>5</sup>; R. Pokorný<sup>4</sup>

1. PNNL, USA
2. AttainX, USA
3. Idaho National Lab, USA
4. UCT Prague, Czechia
5. US DOE, USA

The understanding of batch-to-glass conversion processes aids the development of mathematical models for optimizing batch make-up and process conditions for achieving faster glass production rates. In this study, multiple batch feeds (high-level waste, low-activity waste, and commercial) were analyzed by several experimental methods (feed expansion test, evolved gas analysis, thermogravimetric analysis, and x-ray diffraction) at multiple heating rates. The obtained conversion kinetics data were used to develop kinetic models for the reaction zone of the cold cap (the floating layer of reacting feed on top of molten glass) and to estimate the temperature at the cold-cap bottom, which acts as one of the limiting factors for the heat transfer to the cold cap. These kinetic models were implemented into a large-scale computational fluid dynamics model of a joule-heated melter to estimate the glass production rate of various melter feeds. The modeling results were in good agreement with experimental values from pilot-scale runs and served to quantify the effects of melter operating conditions and feed properties on glass production rates.

10:20 AM

**(GOMD-S4-016-2022) The Effect of Glass Surface Fluidity on Melting Reactions (Invited)**D. R. Swiler<sup>\*1</sup>

1. O-I, R&D, USA

A viscosity equation has been proposed that describes glass as a mixture of strong network bonds and weak internetwork bonds. This equation has fit a wide range of silicate glasses at melting and forming temperatures by modifying only two parameters. For SLS glasses, the equation expressed in Pa•S has the following form:  $\eta(T) = 1 / (0.15(T - T_0) \exp(-E / (T - T_0)))$  Where  $T_0$  is related to amount the ionic internetwork bonding and  $E$  is related to the amount of energy required to break network bonds and form a two dimensional structure. One of the outcomes of this model is the prediction of a higher fluidity at glass surfaces due to interrupted bonding. This fluidity leads to triple point corrosion at the surface of a glass melt, not below as proposed for surface tension induced convection currents. Evaluation of corrosion patterns support the “surface fluidity” model. The presence of these accelerated reaction processes at the surface of glass do not only apply to corrosion of refractories, but to accelerated melting of raw materials in the presence of bubbles. Bubbles that must be removed by the end of the glass melting process may be advantageous inside and below batch piles in conventional SLS glass melting.

10:50 AM

**(GOMD-S4-017-2022) Glass melting and phase separation: Modeling and simulation approaches (Invited)**S. Schuller<sup>\*1</sup>; E. Sauvage<sup>1</sup>; K. Paraiso<sup>2</sup>; A. Cartalade<sup>3</sup>; W. Verdier<sup>3</sup>; S. Gossé<sup>4</sup>; R. le tellier<sup>5</sup>

1. CEA, ISEC/DE2D, France
2. Saint-Gobain Research Provence, France
3. CEA, ISAS/DM2S, France
4. CEA, ISAS, France
5. CEA, IRESNE/DTN, France

Highly focused research programs on nuclear waste vitrification are still underway in the “Science and Technology Institute for Circular Economy of Low Carbon Energies” (CEA/ISEC). The main issues facing us today are to accommodate new types of wastes and higher waste loading, while enhancing the glass quality and increasing the production capacity and robustness of plants. This requires an extensive knowledge on glass melting processes and physical-chemistry of vitreous materials. Basic research supported by a modelling approach is conducted from laboratory-scale and mock-up, to full-scale non-radioactive facilities. This talk will be focused on an academic research conducted to model the glass melting process and the phase separation mechanism in the melt. First a modelling approach able to couple reaction kinetics laws of thermally activated glass melting processes (denitration, crystallization, dissolution) to a magneto-thermo-hydraulic model will be presented. One example of simulation integrating the chemical equation and solved with CFD tools will be presented. Second, we will focus on the phase-field model for the simulation of phase separation mechanism in a ternary phase diagram coupled with real thermodynamic landscape and Navier-Stokes equation.

11:20 AM

**(GOMD-S4-018-2022) Oxidize Sulfate Fining in Borosilicate Glasses**S. M. Jarvis<sup>\*1</sup>

1. Corning Incorporated, USA

Reduced sulfate fining is the most common method of removing bubbles from glass in the container and flat glass industries. Literature suggests high temperature oxidized sulfate fining, while less common, can be effective under the proper conditions. Alumina-borosilicate model glasses were melted with sulfates to investigate the potential of sulfate fining in glass systems traditionally melted at high temperatures.

11:40 AM

**(GOMD-S4-019-2022) Nanoparticle Formation During Production of Copper Borate Glass in Stainless Steel Crucibles**P. N. DeMaere<sup>\*1</sup>; W. Wall<sup>2</sup>; S. Adab<sup>2</sup>; Y. Boluk<sup>1</sup>; C. Calahoo<sup>1</sup>

1. University of Alberta, Civil and Environmental Engineering, Canada
2. Genics Inc., Canada

Furnace materials are typically expensive refractories, yet our low-melting copper borate glasses allow us to use stainless steel crucibles. The reaction between the glass melt with stainless steel presents manufacturing and reliability challenges, but shows a progressive passivation reaction after several melts which results in reproducible melts. The progression of an “unseasoned” crucible to a “seasoned” crucible creates a unique melting condition, i.e., a reducing environment in an oxygen-rich atmosphere. Consequently, different stages of copper reduction and metallic crystal growth were observed, with regions of both brown transparent copper nanoparticles (Cu-NP) and full metallic copper being explored using IR and Raman spectroscopy. The systematic reduction of copper as a function of stainless steel surface condition provides a unique synthesis route for Cu-NP, not unlike that used for the production of colloidal copper glasses manufactured throughout the millennia, such as Purpin and aventurine glass or goldstone. More recently, Cu-NP

## Abstracts

have been utilized in optical applications, surface-enhanced Raman spectroscopy, or as anti-microbial and anti-viral additives, making this synthesis route of modern interest as well. Furthermore, the ability to reliably use stainless steel as a refractory material provides more synthesis options to glass manufacturers.

### Award Lectures

#### Norbert J. Kreidl Award for Young Scholars

Room: Constellation C/D (Second floor)

Session Chair: Charmayne Lonergan, Pacific Northwest National Lab

12:25 PM

#### (GOMD-AW-003-2022) Synthesis, structure and properties of pure TeO<sub>2</sub> glass, binary and ternary tellurite glasses

N. Tagiara<sup>\*1</sup>

1. National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Greece

In the context of the PhD thesis entitled "Synthesis, structure and properties of pure TeO<sub>2</sub> glass, binary and ternary tellurite glasses", we synthesized for the first time pure TeO<sub>2</sub> glass in sizable quantities by melting in Pt crucibles and quenching using our newly developed intermittent quenching technique. 1 Glass transition temperature ( $T_g$ ), density ( $\rho$ ) and elastic properties of pure TeO<sub>2</sub> glass were measured and its structure was studied by Raman and infrared (IR) spectroscopy. 1,2 In parallel, (TeO<sub>2</sub>)<sub>6</sub> and (TeO<sub>2</sub>)<sub>12</sub> clusters were studied by density functional theory (DFT) and the Raman and IR spectra were calculated and compared with the experimental spectra. 3 It was found that (i)  $T_g$ ,  $\rho$ , elastic moduli and structure of pure TeO<sub>2</sub> glass are distinctly different from those reported for TeO<sub>2</sub> glasses melted in alumina crucibles, (ii) pure TeO<sub>2</sub> glass has no Te=O bonds, and (iii) its structure consists of trigonal bipyramidal TeO<sub>4</sub> units connected by asymmetric and nearly symmetric Te-O-Te bridges (as in  $\gamma$ -TeO<sub>2</sub>), and involves also edge-shared TeO<sub>4</sub> units through double oxygen bridges, Te-O<sub>2</sub>-Te, as in the  $\beta$ -TeO<sub>2</sub> polymorph.

### S1: Fundamentals of the Glassy State

#### Glass Formation and Structural Relaxation I

Room: Constellation E (Second floor)

Session Chairs: Sabyasachi Sen, University of California, Davis; Collin Wilkinson, Pennsylvania State University

1:20 PM

#### (GOMD-S1-030-2022) Glasses Prepared by Physical Vapor Deposition (Invited)

J. Gabriel<sup>1</sup>; E. Thoms<sup>1</sup>; R. Richert<sup>\*1</sup>

1. Arizona State University, School of Molecular Sciences, USA

Glasses are usually prepared by cooling the melt, and the final properties can be tuned by the rate at which the material is cooled in the vicinity of the glass transition temperature,  $T_g$ . Glasses that are qualitatively more different from the result of cooling the melt can be obtained by physical vapor deposition (PVD), as recently demonstrated by Ediger and coworkers. PVD onto substrates held at low deposition temperatures ( $T_{dep} \ll T_g$ ) has been used to circumvent crystallization, but using  $T_{dep} \gg 0.85T_g$  instead yields glassy states that would require thousands to millions of years to achieve by physical aging. Such kinetically stable glasses show higher densities, reduced amplitudes of the secondary (Johari-Goldstein) relaxation amplitude, elevated DSC onset temperatures, low entropies and enthalpies, and possibly some anisotropy. The combination of low temperatures and high mobility at the glass/vacuum interface is

responsible for the development of these extraordinary properties, as observed in-situ by dielectric relaxation experiments, which have revealed that a few nanometers of a highly mobile surface layer exists during deposition. Contrary to expectation, glasses prepared by PVD do not necessarily recover the ordinary liquid properties when the temperature is raised to above  $T_g$ . Several examples of such behavior will be shown, using dielectric techniques to characterize the structure and dynamics of the sample.

1:50 PM

#### (GOMD-S1-031-2022) Influence of the modifier type on the surface properties of alkali silicate glasses (Invited)

W. Kob<sup>\*1</sup>; Z. Zhang<sup>2</sup>; S. Ispas<sup>1</sup>

1. University of Montpellier, France

2. Xi'an Jiaotong University, State Key Laboratory for Mechanical Behavior of Materials, China

Understanding and controlling the microscopic properties of glass surfaces are crucial for many applications. However, obtaining this information from experiments is difficult because of limited spatial resolution and/or small probe volume. In this talk we will present the results from atomistic computer simulations in which we have determined the surface properties of alkali-silicate glasses as a function of the alkali type. Two types of glass surfaces are considered: Surfaces obtained by cooling a liquid with a free surface into its glass state and surfaces resulting from a fracture process. We discuss how the various competing mechanisms give rise to a structure that is surprisingly complex as a function of alkali type and production history.

2:20 PM

#### (GOMD-S1-032-2022) Mixed-Alkali Effect on the Fragility and Viscoelasticity of Metaphosphate Glass Forming Liquids

T. Yeo<sup>\*1</sup>; S. Sen<sup>1</sup>

1. University of California, Davis, Materials Science and Engineering, USA

Continuous substitution of one alkali with another is known to result in the so-called mixed-alkali effect (MAE), which is typically characterized by a strong nonlinear compositional variation in the thermal and transport properties of various glass-forming systems such as the glass transition temperature  $T_g$ , ionic conductivity and viscosity. However, systematic investigations of the MAE on the rheological behavior of glass-forming liquids remains largely missing in the literature. In this work the rheological behavior of super-cooled mixed-alkali metaphosphate liquids of general composition  $Li_xNa_{1-x}PO_3$  is studied using oscillatory parallel plate rheometry. The results of this study detailing the MAE on  $T_g$ , fragility and viscoelasticity of these liquids will be reported, and the fundamental nature of this effect will be discussed.

2:40 PM

#### (GOMD-S1-033-2022) The glass formation boundary in aluminosilicates

H. Lee<sup>\*1</sup>; W. M. Carty<sup>1</sup>

1. Alfred University, New York State College of Ceramics, USA

The glass formation boundary defines a chemistry space within which compositions prefer to remain amorphous when cooled from a melt. Work on alkali aluminosilicates and alkaline earth aluminosilicates demonstrated that the alumina edge of the glass formation boundary was defined by a fixed molar ratio of 1.2 ( $\pm 0.1$ ) Al<sub>2</sub>O<sub>3</sub> to 1.0 R<sub>2</sub>O (Na<sub>2</sub>O or K<sub>2</sub>O) or RO (CaO or MgO) over a broad range of silica levels and is independent of cooling rate. These results were consistent with the glass composition in porcelains, the grain boundary chemistry in sintered alumina, and gloss-matte boundary in whiteware glazes with mixed fluxes.

**3:00 PM****(GOMD-S1-034-2022) Evidence of Ionic Relaxation in the Dynamic Light Scattering of Sodium Borate Melts**D. Sidebottom\*<sup>1</sup>; H. Uppala<sup>1</sup>

1. Creighton University, Physics, USA

Dynamic light scattering provides the dynamic structure factor at small wavevectors and reveals both the non-exponentiality and non-Arrhenius character of the  $\alpha$ -relaxation in glass forming melts. Although many studies have been reported in simple molecular liquids, few exist in network-forming oxides where alkali addition can systematically alter the network structure and in so doing influence the dynamics of the melt. Here we report photon correlation spectroscopy measurements conducted on sodium borate glass melts over a range of compositions for which the fragility increases nearly three-fold. In addition to the primary  $\alpha$ -relaxation, we observe an additional relaxation process that we attribute to the diffusion of the sodium ions. This wavevector dependent relaxation traces its origin back to the microscopic hopping of the ion between charge-compensating sites occurring on the same timescale as that of the  $\alpha$ -relaxation.

**Glass Formation and Structural Relaxation II**

Room: Constellation E (Second floor)

Session Chair: Sabyasachi Sen, University of California, Davis

**3:40 PM****(GOMD-S1-035-2022) Regularities in structural development of As- and Ge-based chalcogenide glasses (Invited)**R. Golovchak\*<sup>1</sup>

1. Austin Peay State University, Physics and Astronomy, USA

The structure of chalcogenide network glasses containing As and/or Ge is thoroughly analyzed through the entire glass-forming region using experimental data of high-resolution X-ray photoelectron, extended X-ray absorption fine structure and Raman spectroscopies. It is shown to obey chemically-ordered bond network model based on "chain-crossing" and "outrigger raft" structural motifs if ordinary synthesis procedure is followed. The best match to the criteria of "chain-crossing" model is obtained for  $\text{As}_x\text{Se}(\text{S})_{100-x}$  bulk glasses with  $x \leq 40$  and  $\text{Ge}_x\text{Se}(\text{S})_{100-x}$  glasses with  $x < 12$ . Sulfides, in general, show greater deviations (~20%) from ideal chain-crossing model than selenides. Germanium selenide/sulfide glasses within the  $12 \leq x < 20$  compositional range are described by a mixed chain-crossing and outrigger raft model, which becomes a dominant structural motif in  $\text{Ge}_x\text{Se}(\text{S})_{100-x}$  at  $x \geq 20$ . These regularities in structural development are shown to have a significant impact on the connectivity of glass backbone and the number of constraints per atom. The latter play an important role in structural relaxation of chalcogenide glasses and their susceptibility to physical aging effects. Network modifiers, such as Bi, Ga and Sb are shown to changes chemical bonds distribution from a predicted according to chain-crossing and/or outrigger raft model behavior.

**4:10 PM****(GOMD-S1-036-2022) Structural relaxation in chalcogenide glasses (Invited)**J. Malek\*<sup>1</sup>

1. University of Pardubice, Department of Physical Chemistry, Czechia

Precise volume and enthalpy relaxation studies of various chalcogenide glasses ( $\text{Se}$ ,  $\text{As}_2\text{Se}_3$ ,  $\text{As}_2\text{S}_3$ ,  $\text{Ge-Sb-S}$ ,  $\text{Ge-Se}$ ,  $\text{Ge-Ga-Te}$ ,  $\text{Ge-Se-Te}$  and  $\text{Ge-Te}$ ) were performed by dilatometry and DSC for simple temperature jump, as well as for more complex thermal history. The volume and enthalpy relaxation data can be described by standard Tool-Narayanaswamy-Moynihan (TNM) model. These results are compared with previously reported TNM data ( $\Delta h/R$ ,  $\ln A$ ,  $\beta$ ,  $x$ ) for many inorganic and organic glass-forming systems.

The relaxation rate  $R_f$  is defined as fictive temperature change per decade of time. It can be used for volume and enthalpy relaxation response comparison among different glass-forming systems. It is shown that  $R_f$  is controlled by the non-exponentiality parameter  $\beta$  and the non-linearity contribution (kinetic fragility of supercooled glass-forming liquid at the glass transition combined with  $1 - x$ ). This approach can be used for comparison and prediction of relaxation behavior of chemically dissimilar glass-forming systems. It is shown that the volume and enthalpy relaxation kinetics is quite fast for materials exhibiting small non-linearity contribution such as  $\text{As}_2\text{Se}_3$  and  $\text{As}_2\text{S}_3$  glasses. It seems that volume and enthalpy relaxation processes start to decouple for glassy materials with intermediate non-linearity contribution such as amorphous Se. These experimental findings are analyzed and discussed.

**4:40 PM****(GOMD-S1-037-2022) Revisiting the Adam-Gibbs Equation through Energy Landscape Modeling**C. Wilkinson\*<sup>1</sup>; J. C. Mauro<sup>2</sup>

1. GlassWRX, USA

2. Pennsylvania State University, Department of Materials Science and Engineering, USA

The Adam-Gibbs model is essential to the current understanding of glass physics as it relates macroscopic (experimentally accessible) properties to an underlying thermodynamic quantity, the configurational entropy. The configurational entropy, in turn, is a function of the high-dimensional energy landscape; thus, by understanding the energy landscape direct knowledge of macroscopic properties is obtained. In this talk, we use new developments in the study of energy landscapes to calculate the configurational entropy. This direct calculation then allows for new insights into the nature of glass relaxation as well as for various viscosity models to be compared.

**5:00 PM****(GOMD-S1-038-2022) Non-Arrhenius Viscous Behavior and the Rate of Change of the Energy Landscape Topography**M. C. Beg\*<sup>1</sup>; J. Kieffer<sup>1</sup>

1. University Of Michigan, USA

We conduct a comparative analysis of the mechanical response of a glass forming oxide melt, juxtaposing the adiabatic complex modulus measured at GHz frequencies using Brillouin light scattering and the steady-state shear viscosity measured at zero Hz. We analyze a sodium borate and sodium tellurite glass compositions representing a range of moderate to significant liquid fragilities. We show that the zero- and high-frequency data sets are perfectly compatible with one another by fitting both components of the high-frequency complex modulus using a modified Maxwell-Wiechert model, transforming the loss modulus to viscosity, and extrapolating to zero frequency. We find that this procedure yields an excellent fit to the steady-state viscosity under the condition that we allow for static and relaxational moduli, as well as the activation energy for viscous dissipation to be temperature dependent. This dependence is modulated by the logistic function, which accounts for the structural changes that take place in the material as it transitions from liquid to glass. Accordingly, the fragility of a glass forming liquid can be regarded as a measure to the rate of change in the energy landscape topography.



## Structure of Glasses II

Room: Columbia (Second floor)

Session Chair: Oliver Alderman, STFC

### 1:20 PM

#### (GOMD-S1-039-2022) Effect of the type of modifier on structure and properties of borosilicate glasses – a spectroscopic study (Invited)

D. Möncke\*<sup>1</sup>

1. Alfred University, Inamori School of Engineering at the NYSCC, USA

The structure and properties of glasses of identical modifier/former ratio varies often significantly with the type of modifier cation. After studying structural changes for selected meta-borate and -phosphate glasses by vibrational spectroscopy, we now look into aluminosilicate and boro-silicate glasses. The latter system is not only of technological interest, but also regarding preferential bonding and that the compositional range of sub-liquidus phase separation expands with the field strength of the modifier cation (Cs>Rb>K>Na to Li). Most recently we compared the structure and properties of BK7 type ( $16 M_2O - 10 B_2O_3 - 74 SiO_2$ ) glasses for the full series of alkali ions from M=Cs to Li. Structural analysis of the glasses was based on optical spectroscopy (using Ni as probe ion), Raman, infrared (IR), and nuclear magnetic resonance (NMR) spectroscopy. Substitution of the modifier cations changes not only the equilibrium between trigonal and tetrahedral metaborate units but also the interconnectivity of the borate and silicate groups. While charge deficient  $[B\emptyset_4]^-$  tetrahedra bond preferentially to other borates in low alkali borosilicate glasses, which is reflected in the Raman signature of modified boroxol rings, we now observe the signatures of Danburite and for large cations Reedmergerite rings, reflecting on variations in preferential bonds and the glass network.

### 1:50 PM

#### (GOMD-S1-040-2022) Structural study of alkaline earth aluminosilicate glasses by vibrational spectroscopy

J. L. Hunt\*<sup>1</sup>; R. Youngman<sup>2</sup>; A. Herrmann<sup>4</sup>; E. I. Kamitsos<sup>3</sup>; D. Möncke<sup>1</sup>

1. Alfred University, USA

2. Corning Incorporated, USA

3. National Hellenic Research Foundation, Greece

4. Technical University Ilmenau, Germany

Understanding the structure of alkaline earth aluminosilicate glasses is important for many applications. Through enhanced knowledge of structure property correlations, we could develop commercial glasses for various technologies including damage resistant and stronger glasses for consumer electronics, photonics, nuclear waste sequestration, bio-glasses, and new glasses in life science. Changes in the coordination of aluminate polyhedra, variations in the connectivity of aluminates and silicate units, and the overall degree of polymerization of the network all impact the materials' physical properties. The structure of two alkaline earth aluminosilicate glass series is studied by Infrared, Raman, and UV-VIS spectroscopy. The glasses contain either barium or magnesium oxide as modifier components. Multiple glasses have been prepared for each series with the formula:  $xMO-yAl_2O_3-(100-x-y)SiO_2$ . The aluminum coordination was quantified by  $^{27}Al$ -NMR. The high field strength of  $Mg^{2+}$  compared to  $Ba^{2+}$  has a significant impact on the aluminum speciation as well as on the number of non-bridging oxygen ions in the glasses and therefore also the glass properties.

### 2:10 PM

#### (GOMD-S1-041-2022) Structure and Crystallization in $TiO_2$ -containing Nepheline Glasses

J. McCloy\*<sup>1</sup>; E. T. Nienhuis<sup>2</sup>; N. J. Smith-Gray<sup>1</sup>; J. Marcial<sup>2</sup>; N. C. Hyatt<sup>3</sup>; L. Mottram<sup>3</sup>; M. C. Stennett<sup>3</sup>; C. Le Losq<sup>4</sup>; D. R. Neuville<sup>4</sup>; Y. Zhang<sup>5</sup>; A. Goel<sup>5</sup>

1. Washington State University, School of Mechanical and Materials Engineering, USA

2. Pacific Northwest National Lab, USA

3. University of Sheffield, United Kingdom

4. Institut de Physique du Globe de Paris (IPGP), France

5. Rutgers University, USA

The effect of  $Ti^{4+}$  on nepheline glass ( $NaAlSi_3O_8$ ) is investigated as  $SiO_2$  is replaced with  $TiO_2$ . Traditionally,  $TiO_2$  is considered to be a nucleating agent for silicate crystallization but can also be incorporated into the glass network in large amounts. To determine the effect of  $Ti^{4+}$  on the structure, X-ray and neutron pair distribution function analysis paired with Empirical Potential Structure Refinement were conducted, supplemented with Raman spectroscopy, electron probe microanalysis, and X-ray absorption spectroscopy (including Extended X-ray Absorption Fine Structure, EXAFS). Up to 15 mol%  $TiO_2$  can incorporate into the glass network as a four-fold coordinated species, with a minor contribution of higher coordinated Ti. In compositions between  $NaAlTi_{0.1}Si_{0.9}O_4$  and  $NaAlTi_{0.2}Si_{0.8}O_4$ , EXAFS suggests a second coordination sphere change for Ti, from Ti-Ti to Ti-Al. Raman spectroscopy also suggests that as Ti content increases, the Na environment becomes more ordered. Subsequently, heat treatment was performed, resulting in a majority phase of orthorhombic carnegieite ( $NaAlSi_3O_8$ ) into which a fraction of Ti was incorporated. Excess Ti was expelled as brookite  $TiO_2$ , and in the highest- $TiO_2$  glass ( $NaAlTi_{0.3}Si_{0.7}O_4$ ) there was evidence of  $NaAlTi_3O_8$  (structure akin to freudenbergite), consistent with a change in local coordination of Ti and ordering of the Na environment as seen in EXAFS and Raman.

### 2:30 PM

#### (GOMD-S1-042-2022) Experimental Method to Quantify the Ring Size Distribution in Silicate Glasses and Its Simulation Validation

Y. Shi\*<sup>1</sup>; Q. Zhou<sup>2</sup>; J. Neufeind<sup>3</sup>; M. Bauchy<sup>2</sup>

1. Corning Incorporated, Characterization Science, USA

2. University of California, Los Angeles, USA

3. Oak Ridge National Lab, Neutron Scattering Division, USA

Silicate glasses have no long-range order and exhibit a short-range order that is often fairly similar to that of their crystalline counterparts. As such, the out-of-equilibrium nature of glasses is largely encoded in their medium-range order. However, the ring size distribution—the key feature of silicate glasses' medium-range structure—remains invisible to conventional experiments and, hence, is largely unknown. Here, by combining neutron diffraction experiments and force-enhanced atomic refinement simulations for two archetypical silicate glasses, we show that rings of different sizes exhibit a distinct contribution to the first sharp diffraction peak in the structure factor. Based on these results, we demonstrate that the ring size distribution of silicate glasses can be determined solely from neutron diffraction patterns, by analyzing the shape of the first sharp diffraction peak. This method makes it possible to uncover the nature of silicate glasses' medium-range order.

### 2:50 PM

#### (GOMD-S1-043-2022) Structure, viscosity and mixing in $Li_2O/MO$ ( $M=Mg, Ca, Sr, Ba$ ) silicate glasses and melts

D. R. Neuville\*<sup>1</sup>

1. IPGP, géomatériaux, France

The configurational properties of melts and glasses provide fundamental information needed to characterize magmatic processes. A principal difficulty, however is to link the “macroscopic”



configurational entropy with the structure of melts. This has been done by combining viscometry with Raman spectroscopic structural studies. From the viscosity measurements at low and high temperatures, we have obtained the configurational entropy,  $S_{conf}$  ( $\log h = Ae + Be/TS_{conf}$ , where  $h$  is the viscosity,  $T$  the temperature and  $Ae$ ,  $Be$  two constants). We are using Raman spectroscopy at room temperature between the soda and alkaline-earth silicate melts. For these compositions, we establish some link between the variation of the viscosity, the configurational entropy as the function of chemical composition and the Q species obtained from the Raman spectroscopy. These structural variations are related to the changes in configurational entropy. It is possible, to understand this variation of viscosity and mixing between Li and (Ca, Sr, Mg, Ba) in silicate melts.

### Structure of Glasses III

Room: Columbia (Second floor)

Session Chair: Franck Yvon, CNRS

#### 3:40 PM

##### (GOMD-S1-044-2022) Structure, and Mechanical Properties of Glassy Sulfide Solid Electrolytes (Invited)

K. Ohara<sup>\*1</sup>; A. Sakuda<sup>2</sup>; A. Hayashi<sup>2</sup>

1. Japan Synchrotron Radiation Research Institute, Diffraction and Scattering Division, Japan
2. Osaka Prefecture University, Graduate School of Engineering, Japan

Through recent research and development, some solid electrolytes with ionic conductivity on the order of  $10^{-2}$  S  $\text{cm}^{-1}$  have also been discovered. On the other hand, to obtain satisfactory performance with these solid electrolytes, it is important to construct a suitable interface between the electrode active material and the solid electrolyte in an all-solid-state battery and to maintain the interface during long-term charge-discharge cycles. Attention must also be paid to the mechanical properties, which are closely related to the interface phenomena, and thus the correlation between Young's modulus and glass structure of sulfide solid electrolytes are focused on. In this presentation, we will introduce the details of these results so far.

#### 4:10 PM

##### (GOMD-S1-045-2022) Observation of a Reentrant Liquid-Liquid transition in an Arsenic Sulfide Glass-forming Liquid

B. Yuan<sup>\*1</sup>; S. Sen<sup>1</sup>

1. University of California, Davis, Materials Science and Engineering, USA

A fundamental and much-debated issue in glass science is the existence and nature of liquid-liquid transitions in glass-forming liquids. Here we report the existence of a novel reentrant liquid-liquid transition in a S-rich arsenic sulfide liquid of composition  $\text{As}_{2.5}\text{S}_{97.5}$ . The structural nature of this transition and its effect on viscosity are investigated in situ using simultaneous Raman spectroscopic and rheometric measurements. The Raman spectroscopic data indicate that upon heating significantly above its glass transition temperature (260K), the constituent  $[\text{S}]_n$  sulfur chains in the structure of the supercooled liquid first undergo a  $[\text{S}]_n \rightarrow \text{S}_8$  chain-to-ring conversion near  $\sim 373\text{K}$ . DSC measurements indicate that this structural transition is exothermic in nature. Further heating above 383K alters the equilibrium to shift in the opposite direction towards an endothermic ring-to-chain conversion characteristic of the well-known  $\lambda$ -transition reported in pure sulfur liquid. These liquid-liquid transitions are manifested in a sharp change in the activation energy of viscous flow of the liquid that will be shown to be associated with a positive curvature in the temperature dependence of viscosity.

#### 4:30 PM

##### (GOMD-S1-046-2022) Investigation of the Properties of Fragile Metal Oxide Liquids

R. Weber<sup>\*1</sup>; S. K. Wilke<sup>1</sup>; C. J. Benmore<sup>2</sup>; M. SanSoucie<sup>3</sup>; V. Menon<sup>1</sup>; J. Rafferty<sup>1</sup>; S. Kohara<sup>4</sup>; H. Oda<sup>5</sup>; C. Koyama<sup>5</sup>; T. Ishikawa<sup>5</sup>

1. MDI, USA
2. Argonne National Lab, USA
3. NASA, USA
4. National Institute for Materials Science (NIMS), Japan
5. JAXA, Japan

Molten metal oxides are precursors to functional glass materials for a variety of applications. Understanding of their processing-property-structure relationships is often limited by the difficulty in obtaining accurate thermophysical property measurements on the liquid state. This research used the Japan Aerospace Exploration Agency (JAXA) Electrostatic Levitation Furnace (ELF) on the International Space Station to study molten metal oxides over a wide range of temperatures. Measurements of liquid density, viscosity and surface tension were made for selected molten titanates, aluminates and silicates. The effects of the ionic radius of rare earth oxide additions were investigated by using scandium, neodymium, ytterbium and lanthanum as components of binary compositions. In some cases, the atomic structure of the liquids has been measured over similar temperature ranges to the those used for property measurements. This talk will briefly describe the experimental methods, present results of the measurements, and discuss the data in the context of property and structure evolution in fragile oxide liquids when they are supercooled towards the glass transition. This work is supported by NASA under grants 80NSSC18K0059 and 80NSSC19K1288.

#### 4:50 PM

##### (GOMD-S1-047-2022) Boron coordination change and the fragility maximum in glass-forming liquid lithium borates

O. L. Alderman<sup>\*1</sup>; C. J. Benmore<sup>2</sup>; S. Feller<sup>3</sup>; R. Weber<sup>4</sup>

1. STFC, ISIS Neutron and Muon Source, United Kingdom
2. Argonne National Lab, X-ray Science Division, USA
3. Coe College, USA
4. Materials Development, Inc., USA

We have shown previously that boron-oxygen coordination numbers can be measured with remarkable accuracy using high-energy synchrotron x-ray diffraction, via determination of the mean B-O bond length in the pair distribution function. Herein we apply this technique to molten and glassy lithium pyro- and meta-borates over wide temperature ranges. A simple model based on chemical equilibrium between tetrahedral and trigonal planar borate isomers is developed and fitted to the experimental data, yielding insight into the temperature dependence of configurational heat capacities and entropies. Combined with our earlier data on sodium borates, the influence of the borate isomerization reaction on the compositional trends of configurational heat capacity and liquid fragility are revealed. In particular, a maximum in both properties is predicted at the metaborate composition, in agreement with the scarce available experimental data, and in contrast to more well-known borate anomaly extrema around the diborate composition. Work was supported by U.S. Department of Energy (DOE) grants SBIR DE-SC0015241 and DE-SC0018601, NASA 80NSSC18K0059 (OLGA, RW), & NSF DMR-1746230 (SF). This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

### **S2: Glass and Interactions with Its Environment: Fundamentals and Applications**

#### **Nuclear Waste Immobilization II**

Room: Frederick (Second floor)

Session Chair: Daniel Caurant, Chimie Paristech CNRS

**1:20 PM**

#### **(GOMD-S2-040-2022) Multivariate Analysis: An essential for studying complex glasses**

I. Sargin<sup>\*1</sup>; J. McCloy<sup>2</sup>; S. Beckman<sup>2</sup>

1. Middle East Technical University, Metallurgical and Materials Engineering, Turkey
2. Washington State University, School of Mechanical and Materials Engineering, USA

Understanding the impact of individual compositional components on the devitrification of complex multicomponent glasses typically requires numerous studies to examine each component's impact. Here we apply exploratory data analysis to a heterogeneous data set of silicate glasses to determine the cations' individual and interacting effects on the crystallization of nepheline (nominally NaAlSiO<sub>4</sub>). Our data consisted of 795 compositions of simulated high-level nuclear waste glasses. We determine the interactions in the heterogeneous data that cause deviations from the behavior found in simplified composition studies. Using both univariate and bivariate exploratory data analysis techniques, we demonstrate the importance of including calculated structural glass parameters on nepheline's devitrification, including field strength, cation to anion radius ratio, and single-bond strength. We also show that studies with simplified glass compositions may fall short in generating knowledge directly transferrable to complex glass compositions. The method used in this study has the potential to inform experimental design for simplified compositions that can generate knowledge directly transferrable to complex, multivariable compositions. The observations reported here have broad implications for any study attempting to map the physical properties of a complex glass containing numerous cations.

**1:40 PM**

#### **(GOMD-S2-041-2022) Impact of mixed network former effect on spinel crystallization in high-level nuclear waste glasses**

N. Balasubramanya<sup>\*1</sup>; P. Florian<sup>2</sup>; A. Scrimshire<sup>3</sup>; P. A. Bingham<sup>3</sup>; M. Ahmadzadeh<sup>4</sup>; J. McCloy<sup>4</sup>; M. I. Tuheen<sup>5</sup>; J. Du<sup>5</sup>; S. Kamali<sup>6</sup>; A. Goel<sup>1</sup>

1. Rutgers-The State University of New Jersey, Materials Science and Engineering, USA
2. CNRS, CEMHTI, France
3. Sheffield Hallam University, Materials and Engineering Research Institute, United Kingdom
4. Washington State University, School of Mechanical and Materials Engineering, USA
5. University of North Texas, Department of Materials Science and Engineering, USA
6. Middle Tennessee State University, Department of Physics and Astronomy, USA

The vitrification of nuclear wastes with high Fe, Ni, and Cr fractions often results in the unwanted crystallization of spinels in the Joule heated ceramic melters, posing a threat to its efficiency and potentially limiting waste loading. The study focuses on the impact of the mixed network formers (Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub>, B<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub>, and Al<sub>2</sub>O<sub>3</sub>/B<sub>2</sub>O<sub>3</sub>) in the system Na<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub>-Fe<sub>2</sub>O<sub>3</sub>-MnO-NiO-Cr<sub>2</sub>O<sub>3</sub> where Fe<sub>2</sub>O<sub>3</sub> = 9 mol%. A suite of characterization techniques such as X-ray diffraction (XRD), vibrating sample magnetometry (VSM), differential scanning calorimetry (DSC), Raman spectroscopy, magic angle spinning- nuclear magnetic resonance (MAS NMR) spectroscopy, and Mössbauer spectroscopy has been employed and augmented by

classical molecular dynamic (MD) simulations. The study suggests that with the increasing Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> and B<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> ratios, the compositions have a higher tendency for spinel crystallization, with Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> having a relatively greater impact. These tendencies have been observed to depend upon (i) the preferential charge compensation of the Na<sup>+</sup> amongst the tetrahedral network forming units (Al, B, Fe) in the order Al > B > Fe which leads to an increase in Fe<sup>2+</sup>/ΣFe and, (ii) unmixing of the aluminoborosilicate network taking into account the tetrahedral avoidance rule between [AlO<sub>4</sub>]<sup>-</sup>, [BO<sub>4</sub>]<sup>-</sup> and [FeO<sub>4</sub>]<sup>-</sup>.

**2:00 PM**

#### **(GOMD-S2-042-2022) Impact of non-framework cation mixing on the structure and crystallization behavior of model high-level nuclear waste glasses**

N. Balasubramanya<sup>\*1</sup>; Z. Sun<sup>1</sup>; M. Ahmadzadeh<sup>2</sup>; S. Kamali<sup>3</sup>; D. R. Neuville<sup>4</sup>; J. McCloy<sup>2</sup>; A. Goel<sup>1</sup>

1. Rutgers-The State University of New Jersey, Materials Science and Engineering, USA
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3. Middle Tennessee State University, Department of Physics and Astronomy, USA
4. CNRS, IGP, France

Spinel crystallization is known to be detrimental to the operation of Joule heated ceramic melters during the vitrification of iron rich high level nuclear wastes (HLW) into borosilicate glasses. This study focuses on understanding the relationship between iron redox, composition, and spinel crystallization tendency in a simplified high level nuclear waste focusing particularly on the impact of non-framework cation mixing. Glasses and glass-ceramics in the Na<sub>2</sub>O-M<sub>2</sub>O-Al<sub>2</sub>O<sub>3</sub>-B<sub>2</sub>O<sub>3</sub>-Fe<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> system (M = modifier cation, in this case, Li or Ca), with varying CaO/Na<sub>2</sub>O and Li<sub>2</sub>O/Na<sub>2</sub>O ratios, have been synthesized by melt quench technique and studied for their crystallization behavior. The resulting interplay between Fe<sup>3+</sup> and other tetrahedrally coordinating elements (Si, B) have been studied by a suite of characterization techniques such as X-ray diffraction (XRD), vibrating sample magnetometry (VSM), differential scanning calorimetry (DSC), Raman spectroscopy, and Mössbauer spectroscopy. Scanning electron microscopy (SEM) and Energy dispersive spectroscopy (EDS) have been employed to understand the crystalline phase distribution in the glass-ceramic samples. The results demonstrate that in a system with Na<sup>+</sup> as the only alkali, spinel crystallization is reduced, but the tendency to crystallize increases significantly when Na<sup>+</sup> is replaced with Li<sup>+</sup> or Ca<sup>2+</sup>.

**2:20 PM**

#### **(GOMD-S2-043-2022) Insights into the of iron and phosphorus induced structural disorder in sodium aluminoborosilicate glasses and its impact on their melt rheology and crystallization behavior**

Y. Zhang<sup>\*1</sup>; N. Balasubramanya<sup>1</sup>; N. Stone-Weiss<sup>2</sup>; S. Kamali<sup>3</sup>; R. Youngman<sup>2</sup>; P. Florian<sup>3</sup>; A. Goel<sup>1</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Corning Incorporated, USA
3. CNRS, France
4. University of Tennessee Space Institute, USA

As being an important component in Hanford high-level nuclear waste (HLW) glasses introduced by bismuth phosphate process, P<sub>2</sub>O<sub>5</sub> can have significant impact on the structure, crystallization, and redox equilibria of glass systems due to its ability to form bonds with both aluminum and boron, as well as to compete with iron for charge compensator in the glass structure. Only few studies have been carried on the model HLW glasses. Therefore, the present study is focused on understanding the impact of P<sub>2</sub>O<sub>5</sub> on the redox chemistry, structural change and crystallization behavior in the designed crystallization field of nepheline. Three series of glasses

which vary both  $\text{Fe}_2\text{O}_3$  and  $\text{P}_2\text{O}_5$  concentration in the system  $\text{Na}_2\text{O}-\text{Al}_2\text{O}_3-\text{B}_2\text{O}_3-\text{P}_2\text{O}_5-\text{Fe}_2\text{O}_3-\text{SiO}_2$  have been investigated. Raman, Mossbauer and NMR spectroscopy have been used to understand the structure of glass samples. High-temperature viscosity measurements have been performed to understand the impact of iron and phosphorus on the rheology and fragility of glass melts. The results will be discussed in the presentation.

### 2:40 PM

#### (GOMD-S2-044-2022) Does CaO suppress nepheline crystallization in high-level waste glasses?

Y. Zhang<sup>\*1</sup>; R. Youngman<sup>2</sup>; A. Pedone<sup>3</sup>; M. Bertani<sup>3</sup>

1. Rutgers University, Material Science and Engineering, USA
2. Corning Incorporated, USA
3. University of Reggio Emilia, Italy

Our understanding of the impact of CaO on the propensity of nepheline crystallization in sodium- and alumina-rich high level waste glasses is ambiguous. The literature on this subject can be divided into two parts, where one section reports its suppressing effect on nepheline crystallization, while the second part of the literature reports the opposite. The current work aims at solving this mystery and unearthing the underlying drivers governing the effect. Accordingly, two series of glasses in the  $\text{Na}_2\text{O}-\text{CaO}-\text{Al}_2\text{O}_3-\text{B}_2\text{O}_3-\text{SiO}_2$  system, namely Ca-x and NC-y series, have been investigated based on their optical basicity values. In Ca-x series, the CaO content has been increased from 0 to 15 mol.% while maintaining the molar ratio of all the other oxides constant. In NC-y series, the CaO/Na<sub>2</sub>O ratio has been varied. The structure of the as-synthesized glasses has been investigated using state of art (MQ) MAS NMR and Raman spectroscopies in conjunction with MD simulations, while CCC tests have been employed to study the impact of CaO on nepheline crystallization in the glasses. Based on the results obtained, it is evident that CaO does not suppress nepheline crystallization in Ca-x series. The trend observed in NC-y series, however, is completely opposite. The correlation between the short-to-medium ordering in the glass structure and crystallization behavior will be discussed in the presentation.

### 3:00 PM

#### (GOMD-S2-045-2022) Diopside Crystallization in A Simulated HLW Glass

R. Jia<sup>\*1</sup>; C. Niu<sup>1</sup>; Z. Jia<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State key Laboratory of Silicate Materials for Architectures, China

Borosilicate glasses are still today the only kind of waste form for industrial immobilization of HLW, while the glass with a high concentration of alkali earth elements could form diopside crystal in the melt, since the light elements, such as Na and B would volatilize during the idling of melter, causing deleterious impacts on discharging nozzle and chemical durability of the glass. Composition is quite vital to the structure and properties of the glass. Thus, this work mainly studied the effect of several key elements, including volatile B and alkalis, alkali earths and transition metals on diopside crystallization behavior in a simulated HLW glass. The glass samples with different concentrations of key elements were heat treated under series of schedules varied in time and temperature. The relations between the size of diopside and concentration, heat-treatment time and temperature were obtained, and the kinetics of diopside crystallization in the glass was discussed.

### 3:40 PM

#### (GOMD-S2-046-2022) Chemical durability assessment of enhanced low-activity waste glasses through EPA method 1313

J. Marcial<sup>\*1</sup>; J. Neeway<sup>1</sup>; C. Pearce<sup>1</sup>; J. Vienna<sup>1</sup>; L. Nava-Farias<sup>1</sup>; C. L. Thorpe<sup>2</sup>; C. L. Corkhill<sup>2</sup>; R. J. Hand<sup>2</sup>; D. Kosson<sup>3</sup>; R. Delapp<sup>3</sup>; A. A. Kruger<sup>4</sup>

1. Pacific Northwest National Lab, USA
2. University of Sheffield, United Kingdom
3. Vanderbilt University, USA
4. U.S. DOE Office of River Protection, USA

The Glass Leaching Assessment for Durability (GLAD) program seeks to develop new strategies to understand the chemical durability of nuclear waste glasses for the disposal in near-surface conditions. Our new experimental findings on the application of the United States Environmental Protection Agency (EPA) Leaching Environmental Assessment Framework (LEAF) EPA method 1313 to low-activity nuclear waste (LAW) glasses will be presented. The EPA method 1313 is a tumbled test using glass powders immersed in different pH solutions at room temperature. The rate of glass alteration calculated from elemental release into solution during a EPA method 1313 test will be compared to the 200°C vapor hydration test (VHT) and the 90°C product consistency test (PCT). The EPA method 1313 provides a high degree of reproducibility and offers the potential to vary solution conditions. Additionally, a linear compositional-property model of elemental release data and pH dependence was developed which was informed by machine learning techniques to predict the glass durability response in the EPA method 1313 from glass composition.

### 4:00 PM

#### (GOMD-S2-047-2022) Structural Integrity of Residual (SIR) Glass Model to Augment Nuclear Waste Glass Design

J. Amoroso<sup>\*1</sup>; D. L. McClane<sup>1</sup>; M. Hsieh<sup>1</sup>; A. A. Kruger<sup>2</sup>

1. Savannah River National Laboratory, USA
2. US Department of Energy, Office of River Protection, USA

Description of a new model based on glass structure considerations to allow for higher waste loading in nuclear waste glasses while maintaining acceptable chemical durability is presented. The model is derived by partitioning the glass composition into theoretical crystalline phases anticipated to be observed during devitrification along with the resultant residual glass. An empirically derived relationship based on maintaining the computed residual glass structure, as determined from non-bridging oxygen content, can successfully filter glasses with acceptable durability. The proposed model, termed the Structural Integrity of Residual (SIR) can successfully identify durable glass compositions containing 20-35 wt%  $\text{Al}_2\text{O}_3$ , a concentration that would allow for increases to the projected waste loading in glasses processed at the Hanford Tank Waste Treatment and Immobilization Plant. Development of the SIR glass model and results of its application will be presented.

### 4:20 PM

#### (GOMD-S2-048-2022) Characterisation of vitrified Scottish hillfort materials from a nuclear-waste glass analogue perspective

J. T. Mansfield<sup>\*1</sup>; C. L. Corkhill<sup>1</sup>; M. T. Harrison<sup>2</sup>; R. J. Hand<sup>1</sup>

1. The University of Sheffield, Department of Materials Science and Engineering, United Kingdom
2. National Nuclear Laboratory, United Kingdom

Long-term glass dissolution underpins the safety of nuclear waste disposal and may be investigated via analysis of analogous glasses that have been exposed to nature for extended durations. Glasses formed during the vitrification (burning) of ancient hillforts are valuable from this perspective, particularly where these glasses occur at high-precipitation sites such as at Dun Deardail (Scotland, UK). The timber-laced stone walls of this hillfort were ignited and melted in ~310 BC; meaning the resulting glass-containing mass has potentially been water-exposed for >2,000 years. This material has been



characterised via X-Ray Diffraction (XRD), Raman Spectroscopy, Scanning Electron Microscopy with Element Dispersive X-Ray spectroscopy (SEM-EDX) and X-ray Computed Tomography (XCT). A vitro-crystalline form was observed, comprising an alkali-aluminosilicate glass with magnetite, quartz and plagioclase feldspar. Fractured relic quartz indicate melting temperatures of 1000-1100 °C, with metallic iron spherules implying reducing conditions during melting. Iron-rich vesicle rims evidence phase separation or precipitation from a pore fluid. A surface layer of lower density than the glass was observed in XCT and a qualitative analysis of this implies that it was preferentially formed on groundwater-accessible surfaces, thereby providing potential evidence of aqueous glass alteration.

**4:40 PM**

### **(GOMD-S2-049-2022) Vitrification of Radioactive Glass Fiber from Nuclear Facilities**

G. Fang<sup>\*1</sup>; X. Zhao<sup>1</sup>; K. Xu<sup>1</sup>

1. Wuhan University of Technology, State Key Laboratory of Silicate Materials for Architectures, China

High efficiency particulate air (HEPA) filters, mainly made of glass fiber, have been widely used in nuclear facilities for ventilation systems. Nuclear contaminated glass fiber should be compressed to reduce the volume and solidified prior to disposal. Vitrification is a world acceptable technology to immobilize the nuclear wastes, owing to the high volume reduction factor and the excellent chemical durability of the glass waste-form. However, nuclear contaminated glass fiber is not yet re-melted to reduce the volume and immobilize nuclides in a nuclear waste melter, because of the higher melting temperature. Thus, this work concentrates on the formulation of waste glass fiber to adapt to the melting process of the current nuclear waste melter. A three-component (glass fiber-CaO-Na<sub>2</sub>O) constrained-region mixture experiment was design and their viscosity data was mainly studied. The quadratic Scheffé model was used to plot component effect on melting temperature. In addition, the retention of simulated nuclides, such as Co, Sr and Cs in the formulated glasses were studied.

## **S3: Optical and Electronic Materials and Devices: Fundamentals and Applications**

### **Charge and Energy Transport in Disordered Materials**

Room: Constellation F (Second floor)

Session Chair: Caio Bragatto, Coe College

**1:20 PM**

### **(GOMD-S3-021-2022) Improved storage of electric power (Invited)**

M. Braga<sup>\*1</sup>

1. University of Porto, Engineering Physics Department, Engineering Faculty, Portugal

Improved storage of electric power will be required in the upcoming era of the Internet of Things (IoT), wireless sensor networks that monitor, detect, and gather data will be vital for advancements in human health, public safety, industrial automation, and energy management. Presently, rechargeable batteries are used to power the wireless network. However, the limitations of today's Li-ion batteries make this power source unfeasible, from a cost, and environmental perspective. Here we show an energy storage cell based on a Na<sup>+</sup>-ferroelectric glassy electrolyte (Na<sub>2.99</sub>Ba<sub>0.005</sub>OCl) that spontaneously reduces its internal resistance while increasing its dielectric constant from -30 to 75°C. This cell forms a negative capacitance capacitor at the interface with the negative electrode while discharging with a load and self-charges for months even while withstanding a load.

The latter cell architecture is suitable for structural applications as it withstands 1.75 kN in the three-point bending mechanical flexural tests while performing electrochemically. The beam-like power cell reached an energy density of 989 Wh.kg<sup>-1</sup> for the positive electrode only (Cu) and an energy density of 78.1 Wh.kg<sup>-1</sup> and specific energy of 86.0 Wh.L<sup>-1</sup> for the active electrolyte (Na<sub>2.99</sub>Ba<sub>0.005</sub>OCl), that drops to 38.0 Wh.kg<sup>-1</sup> and 56.2 Wh.L<sup>-1</sup> for the whole cell (Al/Na<sup>+</sup>-electrolyte/Cu) including the carbon fiber reinforced plastic (CFRP) structural element.

**1:50 PM**

### **(GOMD-S3-022-2022) Elucidating Li's Role in the Architecture of Active Li-ion Cells with Neutron Depth Profiling**

J. L. Weaver<sup>\*1</sup>

1. National Institute of Standards and Technology, Material Measurement Laboratory, USA

Neutron Depth Profiling (NDP) is a non-destructive analysis method for quantitatively mapping Li distribution within Li-ion batteries. Recent NDP/Li-ion battery studies have included in situ mapping of high impedance zones in glassy, solid-state cells, and its use in calculating a more accurate diffusion rate constant for Li in Sn. In both studies the processing of NDP data was confounded by NDP's unique sensitivity to material density. This challenge was overcome by using the Li areal density (in Li atoms cm<sup>-2</sup>) NDP profiles along with data collected by other techniques to develop interpretations of material chemistry. In the first study above, the NDP profiles indicated that most irreversible density changes occurred during the first charge/discharge cycle and corresponded to cell formation. In the second study, diffusion of Li into Sn at a constant potential resulted in a Li concentration gradient. This is consistent with past findings and made assignment of sections of the profiles to select Li<sub>x</sub>Sn stoichiometries difficult. The diffusion constant values were thus calculated by integrating regions of the areal density NDP profiles. In both cases, questions of material densities resulted in an increase in the uncertainty of the final values. Accurate estimation of such uncertainties is the topic of future research.

**2:10 PM**

### **(GOMD-S3-023-2022) Effects of oxy-silicate dopants in Li<sub>2</sub>S - SiS<sub>2</sub> based glassy solid-state electrolyte systems**

J. Wheaton<sup>\*1</sup>; S. Leland<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, Materials Science and Engineering, USA

Glassy solid-state electrolytes based on the 60 Li<sub>2</sub>S + 40 SiS<sub>2</sub> series have been studied extensively for the last 30 years and have shown promising qualities such as modest electrochemical stability, high intrinsic ionic conductivity, and ease of processability. While previous studies have looked at the effects of lithium ortho-oxysalt dopants, few studies have compared the effects of dopants of Li<sub>x</sub>SiO<sub>y</sub> compounds. In this study, various compounds were doped into the Li<sub>2</sub>S - SiS<sub>2</sub> system to increase the glass formability, crystallization resistance, and ionic conductivity of the sulfide glasses. Glasses were fabricated using a melt-quenched technique, with dopant compounds chosen to be at eutectic points in the Li<sub>2</sub>O - SiO<sub>2</sub> phase diagram. Differential scanning calorimetry experiments were conducted to determine the glass transition and crystallization temperatures. Electrochemical impedance spectroscopy (EIS) was used to determine the temperature dependent ionic conductivity. In addition, the electrochemical stability of the glasses was determined through EIS of symmetric cells against lithium metal at no applied voltage and through galvanostatic cycling experiments.



2:30 PM

**(GOMD-S3-025-2022) Preparation and characterization of new Li-Si-P-S-O-N glasses: Comparison of the effects of different starting materials**V. M. Torres<sup>\*1</sup>; P. J. Philipp<sup>1</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, Materials Science and Engineering, USA

Lithium glassy solid electrolytes (GSEs) are promising materials that may lead to the development of solid-state batteries. In our studies to develop and characterize Li-Si-P-S-O-N GSEs, we have prepared glasses in the compositional series  $58\text{Li}_2\text{S} + 31.5\text{SiSi}_2 + 10.5[(1-x)\text{LiPO}_3 + x\text{LiPON}]$  ( $x = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5$ ) using traditional melt quenching techniques. In particular, we have investigated the roles that different forms of  $\text{LiPO}_3$  and  $\text{LiPON}$  have upon the properties and structures of GSEs in this series. Differential scanning calorimetry (DSC) was used to determine the glass transition and crystallization temperature of these glasses. Fourier transformation-infrared (FTIR) and  $^{29}\text{Si}$  &  $^{31}\text{P}$  Magic Angle Spinning NMR (MAS NMR) spectroscopies were used to identify the role nitrogen plays on the glass structure. X-ray Photoelectron Spectroscopy (XPS) was conducted on the glasses to further understand the bonding environment of nitrogen. Data showcases that there is nitrogen present in  $x=0$  when there is no  $\text{LiPON}$  added. Therefore, there is nitrogen present in the starting materials which impact the electrochemical and thermal properties of these materials.

2:50 PM

**(GOMD-S3-027-2022) Correlating thermal conductivity of oxide glasses with modal characteristics and network topology**S. S. Sørensen<sup>\*1</sup>; P. P. Cielecki<sup>4</sup>; H. Johra<sup>3</sup>; M. Bockowski<sup>2</sup>; E. Skovsen<sup>4</sup>; M. M. Smedskjaer<sup>1</sup>

1. Aalborg University, Department of Chemistry and Bioscience, Denmark
2. Institute of High-Pressure Physics Polish Academy of Sciences, Poland
3. Aalborg University, Department of the Built Environment, Denmark
4. Aalborg University, Department of Materials and Production, Denmark

Thermal conductivity is a notoriously difficult material property to predict, especially in disordered materials due to the contributions from both diffusive, propagative, and localized vibrational modes. However, recent advances in understanding thermal conduction from lattice dynamics has unified several theories of conduction, enabling decomposition of the modal contributions to thermal conductivity. Building on these advances, we investigate the thermal conductivity of densified  $30\text{CaO}-10\text{Al}_2\text{O}_3-60\text{SiO}_2$  glasses using experiments and molecular dynamics simulations. Through harmonic and anharmonic lattice dynamics, we find that the computed thermal conductivity matches the experimental results of the as-made glass. This allows us to probe the connection between modal heat conduction, glass structure, and vibrational characteristics of the densified calcium aluminosilicate glasses. We show that vibrations of oxygen, silicon, and aluminum atoms are the main heat carriers, but that their pressure dependencies vary greatly. Furthermore, we observe a strong correlation between the thermal conductivity and the position of the boson peak. Our results provide new insight to the thermal conduction of an archetypical oxide glass system and showcase how the recent advances within lattice dynamics are helpful for characterizing thermal conduction in disordered materials.

Wednesday, May 25, 2022

**Award Lectures****Varshneya Glass Science Lecture**

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

8:10 AM

**(GOMD-AW-004-2022) Chalcogenide optical materials: A 'coming of age' story**K. A. Richardson<sup>\*1</sup>

1. University of Central Florida, College of Optics and Photonics, Dept. of Materials Science and Eng., USA

Chalcogenide materials have been employed in infrared optical systems for decades, but it only within the past several years that chalcogenide glasses (ChGs) and alloys have found their way into designs of optical systems at a scale that enables their transition to the marketplace for broader use in diverse bulk (free-space) and integrated (planar) photonic applications. With their versatile design flexibility in both composition and form factor, ChGs, glass ceramics and phase change alloys are being widely adapted for a range of applications where legacy materials like Germanium, no longer can serve as a cost effective and sustainable option. This lecture describes the attributes of ChGs and their alloys and the market opportunities that are pulling these materials out of the lab onto the commercial stage.

**S1: Fundamentals of the Glassy State****Improved Methods for Glass Structure Determination**

Room: Constellation F (Second floor)

Session Chair: Sushmit Goyal, Corning Incorporated

9:20 AM

**(GOMD-S1-048-2022) Solving structural puzzles in amorphous materials by combining first-principles and machine learning molecular dynamics (Invited)**G. Ori<sup>\*1</sup>

1. Institut de Physique et Chimie des Matériaux de Strasbourg (IPCMS), CNRS | Univ. Strasbourg, France

In the last decades, first-principles molecular dynamics (FPMD) has been a key method in molecular modelling, allowing the accurate description of complex amorphous materials for which classical empirical potentials could only offer qualitative results. In recent years, with the growing development and successful application of machine learning potentials (MLP) with first-principles accuracy, the knowledge achieved thanks to FPMD has been exceptionally extended, giving access to larger sizes and times scales. In this talk, I will present a few cases for which the combination of FPMD and MLP has been crucial in comprehending complex amorphous materials such as glassy chalcogenides and oxyhalides. These two classes of materials show an extensive portfolio of uses in many fields, from advanced memory devices to energy applications. A combined FPMD|MLP approach allows exploring into the detail and with a quantitative prediction power the structural order, dynamics, bonding and electronic properties of such materials with an unprecedented level of understanding.

9:50 AM

### (GOMD-S1-049-2022) A NMR-Driven Reverse Monte Carlo Study of Sodium Borate Glasses

T. Charpentier<sup>\*3</sup>; E. Chesneau<sup>3</sup>; L. Cormier<sup>1</sup>; G. Tricot<sup>2</sup>

1. Sorbonne Université, IMPMC, France
2. Université de Lille, LASIR, France
3. Université Paris-Saclay, CEA, IRAMIS/NIMBE, France

Borate glasses are known to have a large fraction of the boron atoms involved in superstructural units like boroxol or pentaborate rings, in addition to the double coordination of boron atoms (3 and 4). This generates the boron's anomaly, which is a non-linear evolution of properties upon the addition of sodium oxide. In this work, we investigate theoretically and experimentally the structure of sodium borate glasses using <sup>11</sup>B and <sup>23</sup>Na NMR, classical and ab-initio molecular dynamics (MD) simulations and neutron diffraction. We observe that only aiMD produces structural models with a non-negligible fraction of super-structural units (6 membered rings) but still below the one determined by two-dimensional <sup>11</sup>B MQMAS NMR. In order to improve our structural models, in particular to include a larger fraction of superstructural units, we develop a hybrid reverse monte carlo (HRMC) scheme combining MD with NMR and neutron data, taking the fraction of superstructural units as an adjustable parameter. Neutron data are found to be not sufficiently sensitive to discriminate the various structural models, in contrast to <sup>11</sup>B NMR for both BO<sub>3</sub> and BO<sub>4</sub> units (i.e., ring and non-rings species). DFT computations of <sup>11</sup>B and <sup>23</sup>Na 2D MQMAS NMR are in good agreement with experiments.

10:10 AM

### (GOMD-S1-050-2022) Predicting the Dynamics of Atoms in Glass-Forming Liquids by a Surrogate Machine-Learned Simulator

H. Liu<sup>1</sup>; M. Bauchy<sup>\*1</sup>

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

Molecular dynamics (MD) is a workhorse of computational material science. However, the inner-loop algorithm of MD (i.e., numerically solving the Newton's law of motion) is computationally expensive. This is a key limitation since, as a result, MD simulations of glasses are typically limited to very fast cooling rates. Here, we introduce a surrogate machine learning simulator that is able to predict the dynamics of liquid glass-forming systems with no prior knowledge of the interatomic potential or nature of the Newton's law of motion. The surrogate model consists of a graph neural network (GNN) engine that is trained by observing existing MD-generated trajectories. We demonstrate that the surrogate simulator properly predicts the dynamics of a variety of systems featuring very different interatomic interactions, namely, model binary Lennard-Jones system, silica (which features long-term coulombic interactions), silicon (which comprises three-body interactions), and copper-zirconium alloy (which is governed by many-body interactions). The development of machine-learned surrogate simulators that can effectively replace costly MD simulations could expand the range of space and time scales that are typically accessible to MD simulations.

10:30 AM

### (GOMD-S1-051-2022) Improved empirical force field for molecular dynamics simulations of oxide glasses

M. Bertani<sup>\*1</sup>; A. Pedone<sup>1</sup>; M. Menziani<sup>1</sup>

1. University of Modena and Reggio Emilia, Department of Chemical and Geological Sciences, Italy

Oxide glasses play a key role in addressing major global challenges in energy, medicine, and communication systems. The lack of understanding of the composition-structure-properties relationship strongly hampers the development of new glasses with tailored

properties. Classical molecular dynamics (MD) have emerged as a powerful technique to gain insight into this relationship and its accuracy relies on the interatomic potential used. The PMMCS FF, a widely used potential based on two-bodies terms computed with Morse functions, has been improved by the inclusion of three-body interactions and repulsive terms between T-O-T bridges and T-T couples (T = Al, Si, P, B). The obtained BMP force field has also been extended, using Bayesian optimization to fit the parameters, to borate glasses for which the D<sub>e</sub> parameter of the B-O Morse function varies with the composition. The new force field can accurately reproduce the coordination of the cations and the Q<sup>n</sup> speciation of Si, P, Al, and B. It shows very good agreement with the experimental neutron diffraction spectra and allows, thank also to the improved description of the bond angle distributions, to better reproduce the NMR spectra of the active nuclei. Furthermore, the very good description of the network former intermixing allows the reproduction of the mixed alkali effect (MAE) tested on the ionic conductivity of (Na, K)-aluminosilicate glasses.

10:50 AM

### (GOMD-S1-052-2022) Development of a molecular dynamics framework to study the kinetics of thermal poling: Application to sodium silicate glasses

P. Ammu<sup>\*1</sup>; M. Reveil<sup>1</sup>; C. McLaren<sup>1</sup>; N. J. Smith<sup>1</sup>; A. Tandia<sup>1</sup>

1. Corning Incorporated, USA

In thermal poling, an electric field is applied across a glass sample to promote the creation of a network-modifier depleted layer near the anode. This technique can be used to achieve substantial and lasting compositional modifications of glass surfaces, useful for numerous applications. Despite the large amount of accumulated literature, structural re-arrangements occurring near the anode region of glass under thermal poling process are not completely understood. In this talk, I will present our recent effort to develop a new framework to model the kinetics of thermal poling using molecular dynamics (MD). As a case study, I will discuss results for sodium silicates where we predict changes in depletion layer thickness as a function of glass composition, temperature, and applied electric field. I will also discuss structural changes that occur near the anode region during thermal poling as observed in our simulations using this new MD framework.

11:10 AM

### (GOMD-S1-053-2022) Atomic Structure of Amorphous Oxide Thin Films by Fitting to X-ray and Electron Diffraction Datasets

K. Prasai<sup>\*1</sup>; K. Lee<sup>2</sup>; J. Jiang<sup>3</sup>; H. Cheng<sup>3</sup>; R. Bassiri<sup>1</sup>; M. Fejer<sup>1</sup>

1. Stanford University, Applied Physics, USA
2. Sungkyunkwan University, Physics, Republic of Korea
3. University of Florida, Physics, USA

Amorphous oxide thin films have wide ranging applications in areas such as electronics, energy storage and precision optics. Understanding the atomic structure of these films, particularly with respect to fabrication conditions, such as doping and annealing, is a crucial step for optimizing the performance of these applications. In this talk, I will discuss the atomic modeling of thin films of amorphous oxides based on X-ray and electron scattering measurements. I will present a method of using x-ray scattering or TEM measurements of amorphous thin films to generate atomic models by combining it with available interatomic forcefields. I will discuss cases when including both x-ray scattering and TEM measurements can improve the accuracy of atomic models and will present some examples. Example models of pure and doped Ta<sub>2</sub>O<sub>5</sub> and GeO<sub>2</sub> will be presented.

11:30 AM

**(GOMD-S1-054-2022) Structures of niobium-containing silicate glasses from MD simulations with newly developed niobium potential**W. Sun<sup>\*1</sup>; K. J. Veenhuizen<sup>2</sup>; J. Marsh<sup>2</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>1</sup>

1. Lehigh University, Material Science and Engineering, USA
2. Lebanon Valley College, Department of Physics, USA
3. Lehigh University, Department of Physics, USA

Niobium-containing silicate glasses find applications in various technologies. We present a partial charge empirical potential for the Nb-O based on existing parameters of other pairs in a Teter potential to enable molecular dynamics simulations of both lithium niobate crystal and lithium niobosilicate glasses. The obtained potential parameters have been shown to be capable of describing structural features of lithium niobosilicate glasses in a wide composition range, including niobium coordination number and bond length, density, bond angle distribution, polyhedral distribution and fraction of bridging oxygen. The results obtained using this new potential show good agreement with experimental data of density and structure from Raman spectroscopy of lithium niobosilicate glasses and X-ray absorption spectroscopy near Nb K-edge.

11:50 AM

**(GOMD-S1-055-2022) Molecular dynamics simulation of tellurite glasses**A. Jan<sup>\*1</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, India

Tellurium oxide-based glasses are among the most promising candidates for integration in non-linear optical devices, such as up-conversion frequency systems and high speed optical switches. However, these glasses are known to be prone to fast devitrification and hence, it is necessary to understand their formation and properties to be able to take full advantage of their peculiarity. Though a lot of experimental work has been carried out in the field of tellurite glasses but these glasses have not been explored much using atomistic modelling. In this work Tellurium oxide glass has been simulated, using the interatomic potentials based on the framework of Born model of ionic solids and further, core shell model. This work explores the effect of system size, quenching rate, and ensemble (NPT and NVT) in terms of connectivity, short-range and medium range order. The glass is estimated to be sensitive to the quenching rate and ensemble choice but not much to the system size and further this glass is concluded to be weakly connected with the presence of large number of terminal oxygen.

**Non-oxide Glasses and Glass-ceramics I**

Room: Constellation E (Second floor)

Session Chair: Pierre Lucas, Univ of Arizona

9:20 AM

**(GOMD-S1-056-2022) Progress in Hybrid Glass Formation, Characterization and Properties (Invited)**T. Bennett<sup>\*1</sup>

1. University of Cambridge, United Kingdom

The attractive physical properties are heavily employed across the materials spectrum in strikingly diverse applications such as display technologies, photovoltaics, coatings and pharmaceutical packing. On the other hand, porous, crystalline 'hybrid' materials consist of both inorganic and organic components, and contain regions of empty space into which guest molecules can be selectively adsorbed and sometimes chemically transformed. A variety of applications have arisen, including e.g. clean air and water production, drug delivery and the prevention of fruit over-ripening. They are often ordered (crystalline) solids, and order—or uniformity—is frequently held to be advantageous, or even pivotal, to our ability to

engineer useful properties in a rational way. It is surprising that the interdisciplinary area between existing glasses and porous hybrids is almost totally neglected. This is despite the massive opportunities arising from the ability to alter existing glass chemistries with a given set of chemical, and physical properties. This talk introduces a new, 4<sup>th</sup> category of glass material – the hybrid glass – which combines the best of both worlds, and lies in a new area of materials space. Examples are given of their formation, characterisation and potential uses.

9:50 AM

**(GOMD-S1-057-2022) Solution-Processed Telluride Glass for Far-Infrared Applications (Invited)**L. Moghimi<sup>\*2</sup>; P. Wondrak<sup>1</sup>; P. Lucas<sup>1</sup>

1. Univ of Arizona, USA
2. Stanford University, USA

Tellurium-based chalcogenide glasses are materials that are transparent over a range of long infrared wavelengths, making them applicable for many uses such as thermal imaging for civil security as well as chemical sensing. In addition, chalcogenide glasses conceivably have the potential to be 3D printed from glass solutions, which can enable intricate optical designs that are not possible using today's methods. Prior studies have demonstrated that thin films of sulfide and selenide chalcogenide glass can be made from solution and that they retain most chemical, physical, and optical characteristics of the initial glass. Nevertheless, these studies have not been expanded to telluride glasses and solution-based production of telluride glasses with wide infrared optical windows have not yet been reported in the literature. The focus of the study was to bridge this gap by investigating the viability of producing a germanium arsenic telluride chalcogenide glass from solution. The chemical composition, structure, and transmission of the solution-processed telluride sample were measured. The solution-processed sample was found to maintain nearly identical stoichiometry and structure to the source glass, suggesting that the optical properties of the starting glass may also be retained in the solution-processed sample.

10:20 AM

**(GOMD-S1-058-2022) Vitrification of organic semiconductor mixtures with ultralow fragility (Invited)**C. Müller<sup>\*1</sup>

1. Chalmers University of Technology, Sweden

Organic semiconductors are used for a myriad of applications such as light emitting diodes and solar cells. The use of glassy materials is a widely used strategy for ensuring a high degree of device stability. This is because any evolution of the nanostructure of an organic semiconductor tends to affect its optoelectronic performance. This talk will explore how mixing of organic semiconductors influences the tendency to form a molecular glass. A series of perylene derivatives is selected as a model system to investigate the impact of mixing on the kinetic fragility and tendency to crystallize. Mixing of perylenes strongly reduces the kinetic fragility because of a liquid-liquid transition, resulting in an ultralow fragility of only 13 in case of octonary mixtures. The use of glass-forming mixtures may open up a new avenue for the design of more thermally stable organic electronic devices.

10:50 AM

**(GOMD-S1-059-2022) High refractive index IR lenses based on chalcogenide glasses molded by Spark Plasma Sintering**V. Reux<sup>\*1</sup>; L. Calvez<sup>1</sup>; X. Zhang<sup>1</sup>

1. ISCR, France

Alternative way of synthesis for high refractive index tellurides based glasses has been experimented, in addition to low temperature Spark Plasma Sintering. The composition tested, Ge<sub>25</sub>Se<sub>10</sub>Te<sub>65</sub>, has been chosen in the Ge-Se-Te system and characterized. Its index refractive



index of 3.12 and overall optical, thermal and mechanical properties makes it the perfect candidate for IR application. However, due to its relative instability regarding crystallization, formation of GeTe crystals occurs during mechanical alloying using raw elements. Transparency has not been achieved in the sintered samples using this powder, as the crystallization rate is accelerated by the pressure during the process. In parallel, glass samples synthesized by melt-quenching have been used to determine optimal sintering parameters for this composition. The main issue met during those tests has been the carbon contamination, reducing overall transparency of the samples through scatterings. As such, it has been shown that the critical parameter to consider to limiting this pollution is the powder granulometry, needing to be above 100 $\mu$ m for optimal performance. This shows the potential for this method to produce high refractive index IR optics, using even unstable glasses

**11:10 AM**

### **(GOMD-S1-060-2022) Crystallization in glasses in the Ga-Sb-Se ternary system**

L. Verger<sup>\*1</sup>; V. Nazabal<sup>1</sup>; D. Le Coq<sup>1</sup>; L. Calvez<sup>1</sup>

1. Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) – UMR 6226, France

Chalcogenide glasses possess unique combinations of optical, electric and mechanical properties which makes them ideal candidates for a wide variety of applications: infrared (IR) lenses, solid electrolytes, optical fibers, photovoltaic cells, for example. Germanium (Ge) is the most expensive element used in chalcogenide glasses. However, most glasses commercialized for applications in the IR region are composed of this element. This work is dedicated to Ge-free glasses and glass-ceramics. The Ga-Sb-Se ternary has been recently studied. Gallium and antimony in large proportion in chalcogenide glasses usually lead to the crystallization of the melt during the synthesis. Nevertheless, a limited amorphous domain has been found in this ternary. We focus here on five glass compositions belonging to this domain and we study their crystallization behavior by a multi-analytical approach (X-ray diffraction, differential scanning calorimetry, IR and Raman spectroscopies). For all glasses, crystallization of Sb<sub>2</sub>Se<sub>3</sub> and/or Se is detected, even after prolonged annealing time above the glass transition temperature ( $T_g$ ). Gallium thus remains in a glassy environment, whose chemical composition and structure are modified by the formation of Sb<sub>2</sub>Se<sub>3</sub>. The role of Se is investigated and a correlation is made between the Se content in the parent glass, the nature of the crystalline phases and the optical properties of the glass-ceramics.

## **S3: Optical and Electronic Materials and Devices: Fundamentals and Applications**

### **Laser Interactions with Glasses**

Room: Frederick (Second floor)

Session Chair: Casey Schwarz, Ursinus College

**9:20 AM**

### **(GOMD-S3-028-2022) Laser-induced crystallization in glass: The influence of laser specific properties (Invited)**

V. Dierolf<sup>\*1</sup>; C. Au-Yeung<sup>1</sup>; E. J. Musterman<sup>2</sup>; H. Jain<sup>2</sup>

1. Lehigh University, Physics, USA

2. Lehigh University, Materials Science and Engineering, USA

The ability to form single crystals within a glass using focused irradiation with a cw or fs laser has been demonstrated by several groups, worldwide. It opens the possibility to great 3-D architectures for application in integrated photonics. To this end, low-loss optical waveguides, splitter, and other structures have been demonstrated. Moreover, the unique boundary conditions imposed by the laser lead to unique effects such as the rotation of the crystal axis

along and perpendicular to the growth direction. In first order, the spatially selective crystallization process is achieved through localized deposition of energy resulting in localized heating of the sample to temperatures that enable nucleation and growth of a crystal. Other second order effects, such as selective excitation of atomic transitions, and laser properties, such as polarization, have not been considered to the same degree. In this presentation, we will discuss for the Sb<sub>2</sub>S<sub>3</sub> model system how the crystal orientation can be controlled by the polarization of the laser. To elucidate the role of the photon energy on the crystallization process, we will compare result for different laser wavelength, laser beam shapes, and results obtained by other localized heating sources such as X-ray and electron beams.

**9:50 AM**

### **(GOMD-S3-029-2022) Orientability of nanocrystals induced by a laser in oxide glasses (Invited)**

B. Poumellec<sup>\*1</sup>; M. Cavillon<sup>1</sup>; J. Cao<sup>2</sup>; E. Muzi<sup>1</sup>; R. Que<sup>1</sup>; M. Lancry<sup>1</sup>

1. UPSud, SP2M, France

2. Tsinghua University, School of Materials Science and Engineering, China

The mastering of second order non-linear optical properties in the frame of integrated optics requires the control of both morphology and orientation of laser induced crystals. During this talk, we will first describe, with the help of an analytical approach, the thermally related mechanisms involved during laser scanning. This will set our understanding in the contributions played by the mean deposited energy and the scanning speed, on the complex structure of fabricated crystallized line. Then, we will see that the use of most of laser types (CW, pulsed lasers) lead, upon irradiation, to a texture that it cannot be tuned, that is, with the “c” axis parallel to the scanning direction. Conversely, by employing ultrafast (fs) lasers and through a judicious choice of laser parameters, the crystal orientation can be controlled by light polarization when ferro-electric nanocrystals are produced. This will be shown using Li<sub>2</sub>O<sub>3</sub>-Nb<sub>2</sub>O<sub>5</sub>-SiO<sub>2</sub> glass. Moreover, we will show that the addition of B<sub>2</sub>O<sub>3</sub> in the glass allows to enlarge the domain of orientability in the landscape of energy-scanning speed. Finally, due to an organized nanoscale phase separation in the glass during a noncongruent crystallization, one can induce orientable form birefringence, which adds another functionality to the Materials Engineer toolbox. Overall, this work testifies of the many possibilities that ultrafast laser direct writing have to offer.

**10:20 AM**

### **(GOMD-S3-030-2022) Photochemically-Patterned Programmable Large-Area As<sub>2</sub>S<sub>3</sub> Chalcogenide Metalayers for Hybrid Refractive-Diffractive Infrared Media (Invited)**

M. Kang<sup>\*1</sup>; B. Triplett<sup>2</sup>; M. Shalaginov<sup>3</sup>; S. Deckoff-Jones<sup>3</sup>; C. Blanco<sup>1</sup>;

M. Truman<sup>4</sup>; T. Karnik<sup>3</sup>; D. J. McGill<sup>2</sup>; C. Popescu<sup>3</sup>; Y. Zhang<sup>3</sup>; L. Li<sup>3</sup>;

S. An<sup>5</sup>; C. Fowler<sup>5</sup>; C. Schwarz<sup>4</sup>; H. Zhang<sup>5</sup>; A. Agarwal<sup>3</sup>; T. Gu<sup>3</sup>; J. Hu<sup>3</sup>;

C. R. Baleine<sup>2</sup>; K. A. Richardson<sup>1</sup>

1. University of Central Florida, CREOL, College of Optics & Photonics, USA

2. Lockheed Martin Corporation, USA

3. Massachusetts Institute of Technology, USA

4. Ursinus College, USA

5. University of Massachusetts Lowell, USA

Meta-structures bring additional degrees of freedom to manipulate the properties of light propagating through thin flat optical components. Their functionalities rival the traditional bulky counterparts and enable new optical phenomena covering a wide range of spectra from the visible to the terahertz region. Here, we present As<sub>2</sub>S<sub>3</sub>-based surface meta-structures and their optical functionalities for flat optics. The novel two-step photochemical process consisting of direct laser writing and subsequent solution etching enables the fabrication of surface meta-structures with arbitrarily-tunable shapes and a wide range of dimensions on large-area flat platforms.



We utilize a combined computational-experimental optimization to demonstrate hybrid refractive-diffractive media with their outstanding diffraction efficiency. We envision the novel versatile scalable process to provide a better design and fabrication flexibility, thereby opening ways toward new opportunities.

10:50 AM

**(GOMD-S3-031-2022) Structure-Terahertz Properties Relationship in Chalcogenide Glasses: Laser Irradiation**

N. Tostanoski<sup>1</sup>; J. Musgraves<sup>2</sup>; P. Wachtel<sup>2</sup>; S. K. Sundaram<sup>1</sup>

1. Alfred University, USA
2. Rochester Precision Optics, USA

We report early evidence of structure-terahertz (THz) properties relationship for binary arsenic sulfide and arsenic selenide chalcogenide glass systems. Both binary chalcogenide systems had their compositions systematically varied across their respective compositional space, resulting in systematic changes in glass structure, average coordination number, and THz properties. Glass structure information was obtained from Raman spectroscopy. Optical and dielectric properties, including the refractive index, were measured in IR and THz regimes. Terahertz time-domain spectroscopy (THz-TDS) was used to record the real and imaginary optical and dielectric constants across the measured THz bandwidth. Femtosecond laser pulses were used to irradiate the glass samples, modifying the local glass structure and optical properties. Chalcogenide glass structural changes made via laser irradiation are correlated to the THz properties. Linear correlation between visible, far IR, and THz refractive indices are presented.

11:10 AM

**(GOMD-S3-032-2022) Formation and characterization of super-periodic rotating lattice single crystals in glass**

E. J. Musterman<sup>1</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>1</sup>

1. Lehigh University, Materials Science and Engineering, USA
2. Lehigh University, Physics, USA

Controlled lattice curvature can be engineered into crystals grown in glass by local heating through laser irradiation. These metamaterials take advantage of the unique growth conditions imposed by the surrounding glass to create a variety of lattice curvatures which can ultimately lead to super-periodic structures with a superimposed micron scale periodicity. In this presentation, we demonstrate the extended growth of rotating lattice single (RLS) crystal lines to form super-periodic RLS structures in a model system of  $\text{Sb}_2\text{S}_3$  crystals formed in stoichiometric glass. These crystals lines rotate predominantly about an axis perpendicular to the laser scanning direction and parallel to the glass surface, where the axis of rotation tends to align towards two different crystallographic axes with differing periodicities. We use electron backscatter diffraction to characterize the orientation of the initial seeds and lattice rotation. We interpret these results using a dislocation-based model and the characteristic dislocations of the model crystal. Micron scale super-periodic RLS crystal lines as presented in this talk act as another potential metamaterial for novel optical and photonic devices.

11:30 AM

**(GOMD-S3-033-2022) Crystal phase-selective laser-induced crystallization of lead bismuth gallate glass**

K. J. Veenhuizen<sup>1</sup>; O. Magnuson<sup>1</sup>; C. Barker<sup>2</sup>; A. Hearsay<sup>1</sup>; J. Marsh<sup>1</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>3</sup>

1. Lebanon Valley College, Physics, USA
2. Lehigh University, Physics, USA
3. Lehigh University, Materials Science and Engineering, USA

Spatially selective crystallization of glass can be achieved via laser irradiation, allowing for the creation of crystal lines whose optical and electrical properties can be harnessed in opto-electronic devices. Exploiting the inhomogeneous temperature profile and the ability

to tailor it through laser beam shaping and scanning speed, it should be possible to create multiphase structures, allowing a new level of flexibility in designing multifunctional crystal elements. We have tested this hypothesis of phase selective crystallization by laser heating the lead bismuth gallate model glass system, particularly  $50\text{PbO}-40\text{Bi}_2\text{O}_3-10\text{Ga}_2\text{O}_3$  glass. DSC and XRD measurements indicate the formation of multiple crystal phases, a cubic bismuth lead oxide phase at lower temperature and triclinic phase at higher temperature. Laser fabricated crystals in glass were studied using Raman microscopy, within which the presence of both phases was observed for certain laser powers and laser scanning speeds. By varying these processing parameters, phase-selective crystallization of glass was observed, whereby only the cubic phase formed at lower powers and an unknown phase which was not observed during conventional heat treatment formed at lower scanning speeds.

11:50 AM

**(GOMD-S3-034-2022) Formation of Cubic Single Crystal Architecture in Glass Via Femtosecond Laser Irradiation**

C. Barker<sup>1</sup>; E. J. Musterman<sup>2</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>3</sup>; B. Aitken<sup>4</sup>; D. Nolan<sup>4</sup>

1. Lehigh University, Physics, USA
2. Lehigh University, Materials Science & Engineering, USA
3. Lehigh University, International Materials Institute for New Functionality in Glass, USA
4. Corning Incorporated, USA

Devitrification of glass via femtosecond laser allows for the formation of complex single crystal structures in 3D, and opens the way for integrated photonic devices in a glass substrate. Previous work has demonstrated formation of optically active  $\text{LaBGeO}_5$  and  $\text{LiNbO}_3$  single crystals deep inside glasses. However, for certain light emission devices, a cubic host can be advantageous. Additionally, a cubic waveguide system can be more tolerant to variations of crystal orientation, such that losses from birefringence and scattering at unwanted grain boundaries in waveguides are minimized. Motivated by this expectation,  $\text{ZnAl}_2\text{O}_4$  spinel crystals were fabricated in  $\text{ZnO}-\text{Al}_2\text{O}_3-\text{SiO}_2$  glass with a 1026 nm wavelength femtosecond laser focused into the bulk of the glass using a pulse width of 175 fs and a repetition rate of 200 kHz. To control the nucleation rate, the glass was doped with  $\text{TiO}_2$ . Structural changes and morphologies of the modification are characterized by Raman spectroscopy and electron microscopy. Challenges in achieving single crystal growth in a high symmetry cubic system as compared to axially symmetric crystals are discussed.

**S4: Glass Technology and Cross-Cutting Topics**

**Sol-gel Processing of Glasses and Ceramic Materials**

Room: Columbia (Second floor)

Session Chair: Lisa Klein, Rutgers University

9:20 AM

**(GOMD-S4-020-2022) Real-time, Across-length-scale Characterization of Cold Sintering, a Novel Ceramic Processing Technique using Synchrotron Methods (Invited)**

F. Zhang<sup>1</sup>; R. Maier<sup>1</sup>; I. Levin<sup>1</sup>; A. J. Allen<sup>1</sup>

1. National Institute of Standards and Technology, Materials Measurement Science Division, USA

At its most fundamental level, ceramic processing encompasses physical and chemical processes over a range of length scales. A proper understanding of ceramic materials' across-length-scale structural and microstructural evolution is at the core of the structure-property relationship and is essential to process optimization. Traditionally, this goal is accomplished through ex-situ microscopic measurements. Recent advances in high-energy synchrotron X-ray sources enable the real-time characterization of ceramic materials under realistic processing conditions in a continuous size

range from sub-Angstrom to micrometers. This talk will present an overview of the relevant synchrotron-based X-ray scattering and diffraction techniques and their capabilities. We will use our recent study of cold sintering of ZnO as an example. Our synchrotron results, coupled with in-situ monitoring and ex-situ microscopic data, provide insight into the mechanism of cold sintering, a novel pressure-aided low-temperature densification process applicable to many ceramic materials.

9:50 AM

**(GOMD-S4-021-2022) Sol-Gel-Derived Core-Shell GeO<sub>2</sub>-SiO<sub>2</sub> Colloids and Their Application for 3D-Printing Optical Glass (Invited)**

J. F. Destino<sup>\*1</sup>

1. Creighton University, Chemistry, USA

The advancement of additive manufacturing or 3D printing has shown an extraordinary potential to revolutionize many fields, including glass science. We present the development and characterization of silica-encapsulated germania colloids to serve as germania-silica or GeO<sub>2</sub>-SiO<sub>2</sub> particle precursors for fabricating glass by 3D printing. GeO<sub>2</sub>-SiO<sub>2</sub> feedstocks are of interest because silica-germania glasses exhibit similar physical and optical properties to traditional silica glass but with improved optical transmission and a tunable refractive index. Multiple core-shell GeO<sub>2</sub>-SiO<sub>2</sub> hybrid colloid strategies were developed, and the morphology and structure of the resulting particles were characterized by electron microscopy, ATR-FTIR, Raman, XRD, and XPS. Currently, we are investigating hybrid colloids' application and structural evolution from colloids to the printed glass towards understanding how colloid precursor structure influences glass network formation.

10:20 AM

**(GOMD-S4-022-2022) Thermal Insulation Composites Made with Ambient Drying Aerogels (Invited)**

L. Lu<sup>\*1</sup>

1. Liatris Inc., R&D, USA

Buildings and industry combine to consume >70% of the energy in the US, making conservation critical for a greener environment. Liatris is developing next generation of thermal insulation materials addressing both markets that have superior properties versus current thermal insulation products, yet with cost and processing viable for mass production scale. We have successfully developed prototypes which comprises silica aerogel as the main filler and a foamed cementitious material as a binder. This product is the first in a series of organic-inorganic nanocomposite products which have many advantages over traditional insulation products such as polystyrene foams (EPS and XPS), fiberglass, and mineral wool in terms of reduced thermal conductivity, improved mechanical properties, and improved fire resistance properties. Ongoing efforts aim to optimize the composites with clay and nanocellulose reinforced silica aerogels using ambient drying method as opposed to the traditional drying methods such as freeze drying or high pressure supercritical drying. These reinforcements to the aerogel have allowed us to achieve lower shrinkage and higher porosity, a key innovation to enable a new generation thermal insulation products competitive to traditional thermal insulation materials.

10:50 AM

**(GOMD-S4-023-2022) Sol-gel synthesis of a hybrid single ion conducting solid-state electrolyte with double functionalized silica backbone**

G. Wang<sup>\*1</sup>; V. Keshishian<sup>1</sup>; J. Kieffer<sup>1</sup>

1. University Of Michigan, USA

To avoid concentration gradients, cell polarization, and device instability calls for devising single ion-conducting solid-state electrolytes (SSE). We report the development of a novel hybrid SSE consisting

of a porous silica backbone, derived from tetra-ethyl-orthosilicate (TEOS) via sol-gel synthesis. This backbone is then functionalized with 2-[(Trifluoromethanesulfonylimido)-N-4-sulfonylphenyl] ethyl (TFSISPE) anion. Lithium ions are introduced into the system via ion exchange, and finally, samples are immersed into melted PEO (MW = 600), which permeates the network to fill available pore space. The resulting material exhibits a room temperature conductivity of  $1.8 \times 10^{-4}$  S/cm. Conversely, when replacing part of the PEO with 2-[Methoxy(polyethyleneoxy)<sub>n</sub> propyl] trimethoxysilane (Oligo PEO, n=6-9), also covalently grafted to the backbone, the ionic conductivity jumps to  $9.2 \times 10^{-4}$  S/cm. Synthesis of the doubly-functionalized hybrid involves a carefully timed combination of pre-hydrolyzed TFSISPE, oligo PEO, and partially gelled silica, to facilitate anion loading without disturbing the gelation of the backbone. In both cases we observe a lithium-ion transference number of 0.91, which we attribute to the anchoring of the TFSISPE anion. The conductivity increase for the doubly-functionalized hybrid is due to the reduction of osmotic drag.

11:10 AM

**(GOMD-S4-024-2022) Corrosion protection of Magnesium Alloy AZ31B using melting gels obtained with different alkoxy groups**

A. Samateh<sup>1</sup>; M. C. Grzenda<sup>2</sup>; J. Guzman<sup>1</sup>; J. Mosa<sup>4</sup>; L. C. Lei<sup>3</sup>; M. Aparicio<sup>4</sup>; L. C. Klein<sup>5</sup>; J. P. Singer<sup>5</sup>; A. Jitianu<sup>\*1</sup>

1. Lehman College - City University of New York, Chemistry, USA
2. Rutgers University, Department of Mechanical and Aerospace Engineering & Department of Materials Science and Engineering, USA
3. Rutgers University, Department of Mechanical and Aerospace Engineering, USA
4. Instituto de Cerámica y Vidrio, Consejo Superior de Investigaciones Científicas (CSIC), Spain
5. Rutgers University, Department of Mechanical and Aerospace Engineering, USA

Methyl modified melting gels contain methyl groups directly bonded to the silica network which are converted into hybrid glasses at their consolidation temperature. Melting gels were synthesized by the sol-gel method using mono- and di-substituted siloxanes. In this study, two melting gel systems with different compositions have been compared: methyltriethoxysilane (MTES) - dimethyldiethoxysilane (DMDDES) and methyltrimethoxysilane (MTMS) - dimethyldimethoxysilane (DMDMS). Coatings were placed on Mg alloy AZ31B substrates using diluted melting gels with different mono / di-substituted siloxane molar ratios using dip-coating. The SEM evaluation of the cross-sections confirmed good adhesion of the thin coatings. Thickness were about 10 μm for the obtained coating. Structural characterization was performed to analyze the formation of the hybrid network and structural homogeneity throughout the thickness. Mechanical properties were investigated by scratch and micro-scratch tests to evaluate the influence of coatings composition. Electrochemical analysis (Anodic Polarization and Electrochemical Impedance Spectroscopy) has been performed in 0.35 wt. % NaCl solutions, showing a significant improvement of corrosion resistance. The coatings obtained with MTES-DMDDES show a better protection against corrosion of magnesium than the coatings obtained using MTMS-DMDMS.

11:30 AM

**(GOMD-S4-025-2022) Structural Analysis of Proton Conducting Zirconia-Phosphosilicate Hybrid Membranes**

L. C. Joseph<sup>1</sup>; L. C. Klein<sup>\*1</sup>

1. Rutgers University, MS&E, USA

Proton (H<sup>+</sup>) transport in membranes and solid electrolytes leads to their potential use in fuel cells and chemical sensors. Sol-gel oxide composites are a class of materials that exhibit proton conductivity at room temperature and above. The requirements for oxide proton conductors are that they are chemically and thermally stable in the temperature range 200-400°C. At the same time, the oxides

cannot permit gas crossover. To prevent crossover, phenyl triethoxysilane (PhTES) has been substituted for part of the silica in the zirconia-phosphosilicate gels. The amount of substitution and the amount of zirconia have been varied. Effects of the substitutions on proton conduction in dry and humid samples have been measured using impedance spectroscopy and I-V curves. The molecular structure of the gels has been investigated with FTIR, to identify hydroxyls and phenyl groups, and the presence of bridging oxygen bonds. The presence of hydroxyls and water in the structure assists the hopping mechanism for the protons.

## **S1: Fundamentals of the Glassy State**

### **Data-based Modeling and Machine Learning for Glass Science I**

Room: Constellation C/D (Second floor)

Session Chair: Adama Tandia, Corning Incorporated

**1:20 PM**

#### **(GOMD-S1-061-2022) Modelling NMR Spectroscopy of Oxide Glasses with Machine Learning (Invited)**

T. Charpentier<sup>\*1</sup>; Z. CHAKER<sup>1</sup>

1. Université Paris-Saclay, CEA, CNRS, NIMBE, France

Solid-State NMR has now become a key spectroscopy in numerous fields of material sciences. The local environment of each atom is characterized by a NMR fingerprint that can be acquired independently of the crystalline, disordered or vitreous form of the studied material. With recent advances in DFT computations, NMR can now be combined with Molecular Dynamics (MD) simulations to help the interpretation of experimental data. However, such calculations are severely limited in system size by the high-computational cost of DFT computations. In the last years, machine learning (ML) approaches have emerged as powerful methods for accelerating MD and computing materials properties with an accuracy and an efficiency that are close to that of DFT methods and classical MD, respectively. In the specific field of solid state NMR, few approaches have been recently proposed that can be applied to oxide glasses which are complex materials which structural features that are still debated. We describe here an approach based on the concept of atomic-centered descriptors (such as SOAP) combined with Kernel Ridge Regression (KRR) or Artificial Neural Network (ANN) techniques. This enables the prediction of NMR properties for structural models of thousands of atoms. An optimal scheme based on the Least-Square Support Vector Regression algorithm will be presented with applications to simple borate and silicate glasses.

**1:50 PM**

#### **(GOMD-S1-062-2022) Finding Needles in Haystacks: Deciphering a Structural Signature of Glass Dynamics by Machine Learning (Invited)**

H. Liu<sup>1</sup>; M. Bauchy<sup>\*1</sup>

1. University of California, Los Angeles, Civil and Environmental Engineering Department, USA

The complex, disordered structure of glasses makes it challenging to elucidate how their atomic structure control their dynamics. Here, based on molecular dynamics simulations, we adopt machine learning (ML) to interrogate whether a structural signature governing the dynamics of atoms in a glass can be found. We find that the dynamics of glasses is encoded in their static structures. These results establish machine learning as a promising pathway to “find needles in haystacks,” that is, to pinpoint important structural patterns in large complex datasets generated by atomistic simulations.

**2:20 PM**

#### **(GOMD-S1-063-2022) Machine Learning Enables to Predict Glass Properties and Optimize Glass Composition**

T. Han<sup>\*1</sup>; X. Xu<sup>2</sup>; J. Huang<sup>3</sup>; A. A. Kruger<sup>4</sup>; A. Kumar<sup>1</sup>; A. Goel<sup>2</sup>

1. Missouri University of Science & Technology, Material Science and Engineering, USA
2. Rutgers University, Material Science and Engineering, USA
3. Missouri University of Science & Technology, Electrical and Computer Engineering, USA
4. U.S. Department of Energy, Office of River Protection, USA

Glasses have been used for hundreds of years, but some fundamental mechanisms behind glass composition and properties still remain unclear. Researchers usually design new glasses based on the Edisonian trial and error method and expert experience, which is not efficient. In the last two decades, machine learning has emerged as a promising tool to predict material properties and assist in designing new materials. This data-driven method can be employed in glass science and provide new perspectives to conquer current problems in glass design. In this study, we demonstrate several examples where machine learning models can predict glass properties for different applications in a high-fidelity manner. For example, the machine learning models predict mechanical properties, dissolution rate for healthcare purposes, and sulfur solubility for nuclear glasses. Then, the machine learning models optimize the glass composition to achieve targeted properties. Furthermore, the machine learning models quantitatively evaluate the influence of input variables (e.g., mixture design) on predicted properties. Closed-form analytical models that predict glass properties are developed based on the understanding of influential and inconsequential variables. Overall, the machine learning models provide fresh standpoints for understanding and predicting the properties of glasses.

**2:40 PM**

#### **(GOMD-S1-064-2022) Physics-informed data-driven modeling of thermoviscoelastic material behaviors**

A. Vu<sup>\*1</sup>; A. Siva Subramanian<sup>1</sup>; T. Grunwald<sup>1</sup>; T. Bergs<sup>2</sup>

1. Fraunhofer Institute for Production Technology IPT, Fine Machining & Optics, Germany
2. Laboratory for Machine Tools and Production Engineering (WZL) of RWTH Aachen University, Germany

Glass undergoes a glass transition upon heating or cooling runs. In the glass transition, glass strongly exhibits thermoviscoelastic behaviors, which are time- and temperature-dependent. Characterization of viscoelastic responses is the key challenge in developing a physics-based material model. This presentation introduces a data-driven machine learning approach that aims to predict the viscoelastic material responses without performing the characterization experiments. First, a database containing the viscoelastic data of numerous glass variants including chalcogenide, optical, and quartz glasses, was created. Based on the viscoelastic data, a constitutive rheological model was introduced allowing the description of the time- and temperature-dependent responses over the entire temperature range in the glass transition. Finally, a physics-informed neural network model was developed to correlate the underlying physics between the material inputs and the parameters of the constitutive model. The results reveal that the model enables excellent prediction performance of the viscoelastic data when new glasses are introduced to the model. The finding of this work is highly beneficial for glass manufacturers to bypass the costly experimental characterization required for understanding the thermo-viscoelastic behaviors in glass processing.



3:00 PM

## (GOMD-S1-065-2022) Predicting electrical properties of Glasses as a function of composition and wavelengths

M. Zaki<sup>\*1</sup>; J. Jayadeva<sup>2</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, Civil Engineering, India
2. Indian Institute of Technology Delhi, Department of Electrical Engineering, India

Researchers have used machine learning and model explanation methods for predicting and explaining compositional control of electrical properties of glasses: dielectric constant, and electrical conductivity. These properties are known to vary with wavelengths and is an important factor that is required to design glasses for custom electrical applications. In this work, we have used machine learning to predict the two electrical properties as a function of composition and wavelength. We use a dataset of more than 3500 glass compositions and wavelengths and corresponding property values. The feature importance is explained for both the models using the concept of SHAP values giving insight into compositional and wavelength dependence of electrical properties. This will allow researchers to design glasses having specific electrical applications.

## Data-based Modeling and Machine Learning for Glass Science II

Room: Constellation C/D (Second floor)

Session Chair: Adama Tandia, Corning Incorporated

3:40 PM

## (GOMD-S1-066-2022) Learning interaction laws in atomistic system using Lagrangian Graph Neural Networks (Invited)

R. Bhattoo<sup>\*1</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, India

Molecular dynamics simulations are used to realistically simulate the material properties. The interatomic potential energy function (PEF) is critical in determining the validity of the results. Such interatomic PEFs are parameterized using density functional theory (DFT). Usually, interatomic PEF is a multi-body function whose functional form is non-trivial to determine. Therefore, estimating the functional form is critical in determining the interatomic PEF and hence the material properties. Herein, we use Lagrangian Graph Neural Network (LGNN) to learn such interatomic PEF in silica glass system. We show that the LGNN model can learn silica interatomic potential for Si-O, O-O and Si-Si interactions. The inductive bias present in the LGNN makes training easier where it can learn from a significantly small dataset as compared to other ML methods. Thanks to the graph architecture, the size of LGNN model is agnostic to the size of system used and hence, learned LGNN model is scalable. We show the zero-shot generalizability of the LGNN model by simulating systems one orders of magnitude larger than the trained one. Further, LGNN architecture is also capable of incorporating the dissipative force due to connected thermostat. Finally, we show the interpretability of LGNN, which directly provides physical insights on the learned model.

4:10 PM

## (GOMD-S1-067-2022) Bypassing Physics Laws to Simulate Complex Atom Dynamics by Observation-based Graph Networks (Invited)

H. Liu<sup>\*1</sup>; M. Bauchy<sup>1</sup>

1. UCLA, CEE, USA

Atom dynamics governs the dynamical and transport properties of glassy systems. However, simulating many-body dynamics of atoms involves complex (and sometimes unknown) physics laws. This challenges the construction of physics-driven glass simulations that both (i) capture the physics laws and (ii) run with little computation cost. Here, based on graph neural network (GNN), we introduce

an observation-based graph network (OGN) framework to “bypass all physics laws” to simulate complex atom dynamics from pure observations, by taking the example of molecular dynamics (MD) simulations ranging over different families of complex glass systems—which allows us to explore the capacity of OGN simulations that is potentially generic to complex glass dynamics. We find that, solely relying on observing the atoms’ motions, graph networks can learn the underlying physics laws that govern atom dynamics and exhibit powerful predictivity of near-future atom trajectories, regardless of how complex the interatomic interactions are. Notably, the observation-based nature of graph networks enables OGN simulations to bypass numerical constraints of traditional MD simulations (e.g., small timestep), thus leapfrogging the execution speed of MD simulations. Overall, this work thrusts to unlock a new era of modeling dynamical behaviors of complex glass systems by surrogate machine learning simulation engines.

4:40 PM

## (GOMD-S1-068-2022) Low Complexity Neural Network based Accurate Prediction of Glass Properties using Physical and Chemical Descriptors

S. Bishnoi<sup>\*1</sup>; R. Ravinder<sup>2</sup>; N. Krishnan<sup>2</sup>; J. Jayadeva<sup>3</sup>

1. Indian Institute of Technology Delhi, School of Interdisciplinary Research(SIRe), India
2. Indian Institute of Technology Delhi, Department of Civil Engineering, India
3. Indian Institute of Technology Delhi, Electrical Engineering, India

Data-driven regression methods are becoming popular tools for predicting and designing novel materials. In glass, learning properties directly from glass composition is very common. However, these composition-based models are restricted to a particular set of compositions as an input for which they are trained. Herein, we develop physics-based descriptors that can predict the property for any given composition by transforming composition space into twelve universal descriptors space. To this extent, we trained ML models using Low Complexity Neural Network (LCNN) algorithm to learn the descriptor–property relationships for density, Young’s, shear, bulk moduli, thermal expansion coefficient, refractive index, glass transition temperature, liquidus temperature and abbe number having twelve universal descriptors as an input feature. Further, we interpreted these models using SHAP value analysis to understand contribution of descriptors in property value. Overall, these physics-based descriptors combined with LCNN loss prove to be advanced, reliable, and global data-driven models to predict novel glass properties.

5:00 PM

## (GOMD-S1-069-2022) Effects of optimizer and loss function on modeling glass properties with Neural Networks

P. Ammu<sup>\*1</sup>; A. Tandia<sup>1</sup>

1. Corning Incorporated, USA

Neural network (NN) based predictions of properties of oxide glasses is an active and growing area of research. More often, the NN capability is limited due to the availability of data for oxide glasses. In such scenarios, incorporating higher-order optimization functions, such as Levenberg–Marquardt (LM) have revealed better generalizable solutions. In our talk, we will demonstrate the implementation of Levenberg–Marquardt optimizer to develop models to predict properties of glass such as Young’s modulus. In addition, application of predicted residual error sum of squares (PRESS) method as loss function has avoided the overfitting issues. In summary, we will show that coupling of LM and PRESS is critical to building robust models, especially in situations with very limited data size.



5:20 PM

**(GOMD-S1-070-2022) Learning Quantum-accuracy Interatomic Potential for Silica Using Lagrangian Graph Neural Networks**R. Bhattoo<sup>\*1</sup>; N. Krishnan<sup>1</sup>

1. Indian Institute of Technology Delhi, Civil Engineering Department, India

Molecular dynamics (MD) simulations are used extensively to study the complex behavior of glasses. In MD simulations, we use the equations of motion along with time integration to generate atomic trajectories. Due to the small timestep used in simulations, a prohibitively large number of runs are required to perform the melt-quench simulation of glasses, especially when using first principle simulations or density functional theory (DFT). Thus, the MD simulations of glasses rely on empirical interatomic potentials that are fitted from the experiment or DFT simulations data. Thus, the accuracy of any MD simulation is limited by the interatomic potential used in the simulation. Further, fitting the interatomic potential is a challenging process that restricts the applicability of MD simulations to a small family of glasses. To address this challenge, it is imperative to develop a scalable scheme that allows the seamless development of quantum accuracy interatomic potentials for glasses. Here, we propose a novel Lagrangian graph neural network (LGNN) to learn such interatomic potentials for complex glassy systems directly from the trajectory of DFT simulations. We demonstrate it in a silica glass system. We show that the LGNN model can learn silica interatomic potential for Si-O, O-O and Si-Si interactions.

**Glass Crystallization and Glass Ceramics**

Room: Frederick (Second floor)

Session Chair: Matthew McKenzie, Corning Incorporated

1:20 PM

**(GOMD-S1-071-2022) Curved lattices of crystals formed in glass (Invited)**E. J. Musterman<sup>1</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>\*1</sup>

1. Lehigh University, International Materials Institute for New Functionality in Glass, USA

Due to constraints from highly viscous matrix the formation of crystal upon heating of glass is fundamentally different than the one obtained from the cooling of the melt. Formation of often observed voids in the matrix is a macroscopically observed result of confinement, but there are also measurable distortions of the lattice of so formed crystals. For example, uncontrolled bending and twisting of the lattice of spherulitic polycrystalline structures in glass-ceramics have been known for fifty or more years. Only recently it has been possible to obtain macroscopic single crystals with well-defined curved lattice by heating of glass with a focused laser, electron or x-ray beam. By controlling the conditions of irradiation, heating profile and confinement by glass matrix, desired lattice curvature has been introduced reproducibly. Several examples of laser-fabricated single crystals with curved lattices fabricated in glass are compared using a common coordinate system to establish correlations between processing parameters and lattice curvature. The mechanisms of lattice deformations are discussed. The latest developments of laser-fabrication of lattice engineered single crystal architecture in glass are leading to a new class of metamaterials with potential for properties beyond those expected from currently available single crystals.

1:50 PM

**(GOMD-S1-072-2022) In-situ Measurement of Crystallization During Cooling by High Temperature Neutron Diffraction**I. Peterson<sup>\*1</sup>; Y. Shi<sup>2</sup>; Y. Chen<sup>3</sup>; K. An<sup>3</sup>; J. Wright<sup>1</sup>; A. Priven<sup>4</sup>; B. Wheaton<sup>2</sup>; S. Halstead<sup>2</sup>; D. Bogdan<sup>1</sup>

1. Corning Research and Development Corporation, Process Research, USA
2. Corning Research and Development Corporation, Characterization Science and Services, USA
3. Oak Ridge National Laboratory, USA
4. Corning Research and Development Corporation, Glass Research, USA

Crystallization of zirconia from a glass-forming liquid was measured using in-situ neutron diffraction during both heating and cooling. Diffraction data were gathered using VULCAN, the Engineering Diffractometer at the Spallation Neutron Course at Oak Ridge National Laboratory. Several different mathematical approaches to fitting data from non-isothermal experiments are available in the literature. To evaluate these approaches, supplemental data were gathered using in-situ high temperature x-ray diffraction, differential scanning calorimetry and scanning electron microscopy.

2:10 PM

**(GOMD-S1-073-2022) Effect of electric field on glass sinter-crystallization in the  $\text{Li}_2\text{O-SiO}_2$  system**E. B. Ferreira<sup>\*1</sup>; J. R. Murdiga<sup>1</sup>; C. Magon<sup>2</sup>

1. University of São Paulo, EESC, Brazil
2. University of Sao Paulo, IFSC, Brazil

The high temperatures and relatively long time intervals required for sintering have pushed the search for ceramic processing alternatives. One of them, Flash Sintering (FS), boosts ceramic material sintering by applying an electric field, causing abrupt shrinking at temperatures far below the level for traditional sintering. However, FS only recently was achieved with powdered glass compacts. In this case, the enhanced sintering seems to result mainly from over-heating by the Joule effect due to a DC electrical current through the sample. Still, several aspects need to be better understood, such as the chemical composition, chemical depletion, and simultaneous crystallization. We successfully developed an approach for detecting specimen retraction during flash sintering by optical dilatometry in this work. Non-isothermal sintering experiments were performed with and without an electric field for two glass compositions in the  $\text{Li}_2\text{O-SiO}_2$  system:  $\text{Li}_2\text{O} \cdot 2\text{SiO}_2$  ( $\text{LS}_2$ ) and  $\text{Li}_2\text{O} \cdot 2.33\text{SiO}_2$ . The Clusters model was used to fit the relative density data as a function of temperature and track the sinter-crystallization kinetics of an  $\text{LS}_2$  glass. In addition, the heating rates of the  $\text{LS}_2$  sintering specimens were estimated. As a result, different heating regimes were detected, accelerating the viscous flow sintering before the flash event and sharply increasing during it.

2:30 PM

**(GOMD-S1-074-2022) Electron beam heating as a new tool for fabricating novel rotating lattice single crystals in glass**E. J. Musterman<sup>\*1</sup>; V. Dierolf<sup>2</sup>; H. Jain<sup>1</sup>

1. Lehigh University, Materials Science and Engineering, USA
2. Lehigh University, Physics, USA

Local heating by laser irradiation has been demonstrated as a versatile processing method for spatially selective modification and crystallization of glass, including novel rotating lattice single (RLS) crystals. For a given glass, the temperature profile induced by laser absorption is largely dependent on the laser power, wavelength, and absorption mechanism (linear or nonlinear). Electron beam heating offers an alternative route with different temperature profiles given by the absorption physics of electrons. In this presentation, we demonstrate electron beam heating for the local crystallization of  $\text{Sb}_2\text{S}_3$  in Sb-S-I glasses as a model system in both scanning and transmission electron microscopes. We explore the most important

electron beam parameters (accelerating voltage and probe current) and their effect on crystallization. Furthermore, we exploit electron backscatter diffraction for observing locally for the first time in situ transformation of amorphous glass structure to RLS crystal lattice. Understanding and optimizing electron beam heating as given for this model system offers an alternative route for the processing and in situ characterization of spatially selective crystallization of glass.

**2:50 PM**

### **(GOMD-S1-075-2022) What particles and crystals do to the mechanical properties of glass: Case studies**

T. Rouxel<sup>\*1</sup>; P. Houizot<sup>1</sup>; Y. Gueguen<sup>1</sup>; J. Moriceau<sup>1</sup>; T. Lacondemine<sup>1</sup>; P. Sellappan<sup>1</sup>

1. Université de Rennes 1, Glass Mechanics, France

Several examples of glass-ceramics and glass-particulate composites are reviewed, including i) the nucleation and crystallization of Ba<sub>2</sub>Si<sub>3</sub>O<sub>8</sub> spherulites in a barium aluminum silicate glass, ii) the incorporation of gold nanoparticles in a soda-lime-silicate glass, iii) the incorporation of diamond particles in a silicon-oxycarbide glass, and iv) the incorporation of SiC particles in a silicon-oxynitride glass, v) glass-ceramics in the YSiAlON system, and vi) the case of glass particles in a glass matrix. The obtained innovative multi-functional and mechanical properties are first described. Then, the changes of the elastic properties, hardness, toughness and indentation cracking behavior are discussed in the light of microstructure observation.

**3:30 PM**

### **(GOMD-S1-076-2022) Nucleation – The Current State of Affairs (Invited)**

K. F. Kelton<sup>\*1</sup>

1. Washington University, Physics, USA

Controlling nucleation is essential for glass formation and the production of glass ceramics. It is, therefore, of practical importance to develop a fundamental understanding of nucleation processes. The Classical Theory of Nucleation (CNT) provides one common framework that can explain a wide range of steady-state and time-dependent nucleation phenomena. However, CNT is based on several questionable key assumptions, including a sharp interface between the nucleating cluster and the original phase and a one-dimensional kinetic pathway. These and other points will be discussed considering experimental studies in a wide range of systems and a few more advanced theories. Examples of nucleation in silicate and metallic liquids and glasses will be presented to emphasize the importance of ordering in the amorphous structure, which is not included in CNT. A reported failure of CNT to predict the measured nucleation rates in silicate glasses at temperatures below the temperature of the maximum nucleation rate will also be discussed. Finally, some examples of nucleation studies in colloids, biological systems and computer models that point to multiple pathways for nucleation and the effects of stirring will be presented.

**4:00 PM**

### **(GOMD-S1-077-2022) Stress Dependent Phase Transition of Cristobalite Containing Glass-Ceramics**

K. T. Strong<sup>\*1</sup>; T. Diebold<sup>1</sup>; J. Laing<sup>2</sup>; S. Dai<sup>1</sup>; B. Lester<sup>3</sup>

1. Sandia National Laboratories, Material Mechanics and Tribology, USA
2. Sandia National Laboratories, Metallurgy and Materials Joining, USA
3. Sandia National Laboratories, Materials and Failure Modeling, USA

The apparent linear coefficient of thermal expansion of lithium aluminosilicate glass-ceramic (GC) can be tailored by systematically modifying the thermal profile used to crystallize the starting amorphous material. This tunability is useful for applications such as designing and fabricating a matched expansion glass-ceramic to metal (GCTM) seal. Cristobalite is one of the major constituents to crystallize from the glass material, which undergoes an  $\alpha$  to  $\beta$  phase

transition at approximately 220 °C within the GC material. This results in non-linear thermal expansion data. The non-linear expansion behavior can cause thermal-mechanical stresses for GCTM seals. It is necessary to accurately model this transition behavior to accurately predict the residual stresses that can be imparted on joined components. It is well known in the geological community that the behavior of this transition in cristobalite occurs under the pressures of the earth's atmosphere. This study investigates how moderate engineering stresses affect the phase transition of the cristobalite containing GC. Thermal expansion measurements were collected as a function of constant uniaxial applied stress. The results will be compared to a constitutive model developed. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

**4:20 PM**

### **(GOMD-S1-078-2022) Examining the effect of the [SiO<sub>2</sub>]/[Li<sub>2</sub>O] on the microstructure and properties of lithium disilicate glass-ceramics that contain lithium tantalate as a secondary phase**

A. V. DeCeanne<sup>\*1</sup>; C. Ritzberger<sup>2</sup>; M. Dittmer<sup>2</sup>; M. Rampf<sup>2</sup>; J. C. Mauro<sup>1</sup>

1. Pennsylvania State University, Materials Science and Engineering, USA
2. Ivoclar Vivadent AG, Liechtenstein

The present study examines the effect of the ratio of [SiO<sub>2</sub>] to [Li<sub>2</sub>O] on the phase assemblage, microstructure, and corresponding properties of lithium disilicate glass-ceramics that contain lithium tantalate (LT) as a secondary phase. A 15-sample data set was analyzed to study the processing-microstructure-property relationships and validate or disprove a proposed reaction equation from previous work. It was found that LT content increased in the material as [SiO<sub>2</sub>]/[Li<sub>2</sub>O] was decreased, validating the reaction equation. The effect of increased LT content on various properties was examined.

**4:40 PM**

### **(GOMD-S1-079-2022) Driving Crystallization on Silicate Melts through Metadynamics Simulations**

A. Pedone<sup>\*1</sup>; F. Lodesani<sup>1</sup>; S. Urata<sup>2</sup>

1. University of Modena and Reggio Emilia, Italy
2. Ashai Glass Company, Japan

Understanding crystallization mechanism in silica-based materials is of paramount importance to comprehend geological phenomena and for improving technological and industrial processes to design novel materials for a variety of applications. In this communication, we show a remarkable possibility of Metadynamics simulations to drive homogeneous nucleation and crystallization even in highly viscous silicate melts with overcoming the timescale problem of classical Molecular Dynamics simulations. The investigation focused on the nucleation and crystallization processes of  $\beta$ -cristobalite and lithium disilicate crystals from the respective melts, as the first studies to evaluate the free energy landscape for a tectosilicate and a layered crystal precipitating at the atomistic scale. The employment of specific peaks of the partial XRD pattern calculated by considering only silicon ions as collective variables has enabled us to effectively and widely explore the reaction path of the melt-to-crystal transition for the first time.

**5:00 PM**

### **(GOMD-S1-080-2022) Gillespite Glass-Ceramics**

L. Moore<sup>\*1</sup>; M. M. Wallen<sup>1</sup>; G. H. Beall<sup>1</sup>

1. Corning Incorporated, Glass Research, USA

A new type of glass-ceramic based on the rare mineral gillespite (BaFeSi<sub>4</sub>O<sub>10</sub>) has been discovered. Unlike most glass-ceramics, controlling the redox state of the precursor glass proved critical to their preparation. In barium-iron-silicate glasses of stoichiometric composition, internal crystallization of gillespite could only be obtained when most of the iron was in the ferrous state: Fe<sup>2+</sup>:total Fe > 0.5. Otherwise, only surface crystallization was observed. DSC and high temperature XRD showed gillespite crystallization

occurs over a narrow temperature range from 800-850°C with simultaneous formation of sanbornite ( $\text{BaSi}_2\text{O}_5$ ) and cristobalite. Fine-grained glass-ceramics with this phase assemblage were made using Pt as a nucleating agent. Electron microscopy revealed a microstructure of gillespite crystal “rosettes” growing on Pt nuclei with secondary phases filling the intergranular pockets. One interesting feature of these glass-ceramics is their red color, attributed to the unusual square planar configuration of the iron cations in the gillespite crystal structure. A second interesting property of the glass-ceramics is their low thermal expansion. While barium silicate glass-ceramics are well-known for their high coefficients of thermal expansion,  $\text{CTE} > 10 \text{ ppm}/^\circ\text{C}$ , gillespite glass-ceramics with  $\text{CTE} < 3.5 \text{ ppm}/^\circ\text{C}$  have been demonstrated.

## Non-oxide Glasses and Glass-ceramics II

Room: Constellation E (Second floor)

Session Chair: Pierre Lucas, Univ of Arizona

### 1:20 PM

#### (GOMD-S1-081-2022) Combination of theoretical and experimental data to solve the structure of telluride glasses (Invited)

D. Le Coq<sup>\*1</sup>; E. Furet<sup>1</sup>; C. Boussard-Pledel<sup>1</sup>; E. Bychkov<sup>2</sup>

1. University of Rennes, ISCR, France

2. University of Littoral - Côte d'Opale, LPCA, France

Telluride glasses are very attractive due to their unique infrared transparency window compared to other chalcogenide glasses since infrared transparency has already been observed up to 35  $\mu\text{m}$ . The structure of pure chalcogenide glasses is mainly governed by covalent bonding but once other elements such halide, alkaline or earth-alkaline are added, a competition between ionic and covalent bonding occurs. At first, the structure of halide tellurium binary compositions is studied using both molecular dynamics simulations and experimental neutron / X-ray data collected on high-scale facilities. In addition, solid-state NMR experiments and NMR parameter calculations are also shown, and all the investigations are in good agreement with the presence of Te highly coordinated with halogen in these glasses. But, it is also well known that the ionic conductivity of some telluride families can be enhanced by several orders of magnitude upon increasing the content of mobile cations such as  $\text{Ag}^+$ . In this presentation, experimental results showing the crossover between ionic and electronic conductivities in two different families based either on  $\text{As}_2\text{Te}_3$  or  $\text{GeTe}_4$  matrixes will be put forward. Indeed, these experiments coupled with simulated experimental data will be used to propose a structure of these glasses.

### 1:50 PM

#### (GOMD-S1-082-2022) Synthesis and Structural Investigation of Mixed Oxy-Sulfide-Nitride (MOSN) Glasses (Invited)

S. Kmiec<sup>\*1</sup>; J. E. De Souza<sup>2</sup>; S. R. de Souza<sup>2</sup>; S. W. Martin<sup>1</sup>

1. Iowa State University, USA

2. UFGD - Universidade Federal da Grande Dourados, Physics, Brazil

Although difficult to incorporate, nitrogen has been shown to greatly improve the interfacial stability of many solid electrolyte (SE) materials in solid-state batteries, as widely demonstrated by the LiPON compositional family. To expand the understanding of nitrogen in SE materials, mixed oxy-sulfide nitride (MOSN) glasses were prepared by direct ammonolysis of the  $\text{Na}_4\text{P}_2\text{S}_{7-x}\text{O}_x$  (NaPSO) glass series to determine the effects of an isoelectric exchange on the incorporation of nitrogen. The short-range order (SRO) structures in the  $\text{Na}_4\text{P}_2\text{S}_{(7-x)-3/2y}\text{O}_{x-3/2y(1-z)}\text{N}_z$  (NaPSON) glasses were investigated with Raman and infrared (IR) spectroscopies to determine viable reaction pathways for nitrogen incorporation via ammonolysis of oxy-sulfide invert glasses. The N content of the glasses was quantified by CHNS elemental analysis and confirmed through weight change measurements. By combining this information, it was further

possible to determine the anion exchange ratio,  $z$ , for the N substitution of O and S as a function of the base NaPSO glass chemistry,  $x$ . The composition dependent glass transition temperature,  $T_g(x)$ , measured with differential scanning calorimetry (DSC), was found to correlate well with the measured N/P ratio,  $y$ , in the NaPSON glasses.

### 2:20 PM

#### (GOMD-S1-083-2022) Thermodynamic approach to the properties of lithium phosphorus oxynitride glasses

A. López-Grande<sup>1</sup>; F. Muñoz<sup>\*1</sup>

1. Institute of Ceramics and Glass, CSIC, Spain

Oxynitride lithium phosphate-based glasses have been at the center of solid electrolytes research since the development of LiPON amorphous films for microbatteries. The substitution of nitrogen for oxygen produces an improvement in the chemical and mechanical resistance of either bulk phosphate glasses or their amorphous films; and the increased electrical conductivity made then soon appropriate to be applied as solid electrolytes. We are presenting a theoretical approach that could ultimately be used in the design of new electrolytes, which is based on the thermodynamic model of associated solutions from which structure and properties of bulk glasses can be obtained. It is first necessary to estimate the free energy Gibbs values of the stable crystalline lithium oxynitride phosphate compounds within the given phase diagram of interest. Throughout the Latimer approach, one may calculate the entropies of formation of oxynitride compositions and, using the Gibbs-Helmholtz equation, the Gibbs energy of formation can be derived as a function of the O/N substitution in the material. The thermodynamic functions are then used to obtain the equilibrium molar amounts of reaction products from which system properties can be calculated. First results of conductivity of oxynitride phosphates in  $\text{Li}_2\text{PO}_{3.5-1.5x}\text{N}_x$  compositions will be herein presented.

### 2:40 PM

#### (GOMD-S1-084-2022) Elaboration, structure and mechanical properties of oxynitride glasses from the $\text{SiO}_2$ -BaO- $\text{Al}_2\text{O}_3$ - $\text{Si}_3\text{N}_4$ chemical system

A. Duval<sup>\*1</sup>; B. Hehlen<sup>2</sup>; A. Moréac<sup>1</sup>; D. Massiot<sup>3</sup>; P. Houizot<sup>1</sup>; T. Rouxel<sup>1</sup>

1. Université de Rennes 1, France

2. Université Montpellier II, France

3. CEMHTI, MatRMag, France

A specific equipment was designed and built to process and anneal glasses by conventional melting in controlled atmosphere conditions. A series of oxynitride glasses in the  $\text{SiO}_2$ -BaO- $\text{Al}_2\text{O}_3$ - $\text{Si}_3\text{N}_4$  system with up to 27 eq. % N was synthesized in nitrogen atmosphere using BN crucibles (40 g batch) and temperatures ranging from 1500 to 1700 °C, and annealed. The transparency of the glass is retained for nitrogen content up to 9 eq. % N. The atomic organization of the obtained glasses was investigated by Raman scattering and by NMR spectroscopies. The mechanical properties, including hardness, elastic moduli and toughness, are then discussed in the light of the structural characteristics, and in particular of the role of nitrogen on the atomic packing density and network crosslinking.

### 3:00 PM

#### (GOMD-S1-085-2022) Composition, properties, and SRO structures of mixed oxy-sulfide nitride glasses in the series $\text{Na}_4\text{P}_2\text{S}_{7-6x}\text{O}_{4.62x}\text{N}_{0.92x}$ ; $0 \leq x \leq 0.5$

M. P. Martin<sup>\*1</sup>

1. Iowa State University, MSE, USA

Sulfide glassy systems have been studied in detail for their applications as electrolyte materials in all solid-state sodium batteries (ASSB). As pure sulfide chemistries can pose challenges cornering chemical stability, the glasses in the series  $\text{Na}_4\text{P}_2\text{S}_{7-6x}\text{O}_{4.62x}\text{N}_{0.92x}$ ;  $0 \leq x \leq 0.5$  (NaPSON) are studied to show the effect oxygen



and nitrogen have on a phosphate glassy system at a fixed modifier to glass former ratio,  $R$ -value=2. Oxygen and nitrogen were incorporated into the sulfide glass melt through as-synthesized  $\text{NaPO}_{3-3/2y}\text{N}_y$ ;  $y=0.46$  (NaPON) to determine if nitrogen can be incorporated into glass systems indirectly, rather than through ammonolysis. The preparation, properties, and short-range order (SRO) structures of these NaPSON glasses were characterized using DSC, CHNS, XPS, Raman, FT-IR, and NMR spectroscopy. The retention of nitrogen in the glass melt was verified using CHNS, XPS and NMR spectroscopy and proven through changes in thermal properties, including an increase in  $T_g$  and chemical stability for  $x$ -values 0.2-0.3. The SRO structures, characterized with Raman, FT-IR, and NMR spectroscopy, revealed a disproportionation reaction where oxy-nitride species preferentially formed covalent, networking phosphate chains, pushing sodium modifier to the sulfide phosphate glass forming units.

### Predicting Glass Properties

Room: Constellation F (Second floor)

Session Chair: Alfonso Pedone, University of Modena and Reggio Emilia

1:20 PM

#### (GOMD-S1-086-2022) Electronic and vibrational properties of the surface of silica and sodium silicate glasses (Invited)

Z. Zhang<sup>2</sup>; W. Kob<sup>1</sup>; S. Ispas<sup>\*1</sup>

1. University of Montpellier, Lab. Charles Coulomb, France
2. Center for Alloy Innovation and Design, State Key Laboratory for Mechanical Behavior of Materials, China

We use ab initio molecular dynamics simulations to investigate the properties of the dry surface of pure silica and sodium silicate glasses. The surface layers are defined based on the atomic distributions along the direction perpendicular to the surfaces. We show that these surfaces have a higher concentration of dangling bonds as well as two-membered (2M) rings than the bulk samples. Increasing concentration of  $\text{Na}_2\text{O}$  reduces the proportion of structural defects. From the vibrational density of states, one concludes that 2M rings have a unique vibrational signature at a frequency around  $850\text{ cm}^{-1}$ , compatible with experimental findings. We also find that, due to the presence of surfaces, the atomic vibration in the  $z$ -direction is softer than for the two other directions. The electronic density of states shows clear the differences between the surface and interior and we can attribute these to specific structural units. The analysis of the electron localization function allows to get insight on the influence of local structure and the presence of Na on the nature of chemical bonding in the glasses.

1:50 PM

#### (GOMD-S1-087-2022) Indentation Behaviors of Glass Studied by Classical Molecular Dynamics Simulations

H. Liu<sup>1</sup>; L. Huang<sup>\*1</sup>; Y. Shi<sup>1</sup>

1. Rensselaer Polytechnic Institute, Materials Science and Engineering, USA

Despite extensive studies, what controls crack initiation in glass under sharp contact loading remains elusive. The difficulty arises from experimental complexity associated with in-situ investigations at a local scale (tens of microns) under complex and non-uniform stresses. In this context, nanoindentation tests were carried out in classical molecular dynamics (MD) simulations to reveal how the stress field and the glass structure evolve underneath the indenter. Indenter angle and tip radius were varied to study the effect of the indenter sharpness in 2.5-D nanoindentation studies of glasses with and without borons. It was found that a large number of boron atoms in the plastic zone change from three- to four-fold coordination during the loading process, and most of them revert back to the three-fold coordination state during the unloading process. This "reversible" boron coordination change plays a critical role in

increasing the damage resistance of boron-containing glasses. We have further developed a 3-D nanoindentation protocol that can generate cracking patterns closer to those in real-life scenarios. We will show 3-D nanoindentation studies of metallic glasses and oxide glasses, which reveal different pathways for crack initiation and propagation from those observed in previous 2.5-D nanoindentation studies. Stress criteria for crack initiation in 3-D nanoindentation will be discussed.

2:10 PM

#### (GOMD-S1-088-2022) Prediction of Silica Glass Etching with HF Vapor Gas by Kinetic Monte Carlo Simulations

H. Park<sup>\*1</sup>; A. Antony<sup>2</sup>; J. Banerjee<sup>3</sup>; G. Agnello<sup>3</sup>; N. J. Smith<sup>3</sup>

1. Corning Precision Materials, Corning Technology Center Korea, Republic of Korea
2. Corning Incorporated, Manufacturing, Technology, and Engineering Division, USA
3. Corning Incorporated, Science and Technology Division, USA

Understanding surface properties of glass during HF-vapor etching process is essential to optimize treatment processes in various glass-related industries. In this work, we investigate etching mechanism of fused silica glass by HF gas with Kinetic Monte Carlo (KMC) simulation. Detailed pathways of surface reactions between gas molecules and the silica surface with activation energy sets are explicitly implemented in the KMC algorithm for both dry and humid conditions. The developed KMC model successfully describes etching of silica surface with evolution of surface morphology to micron regime. Simulation results show that calculated etch rate and surface roughness are in good agreement with experimental results, and effect of humidity on the etch rate is also confirmed. Development of roughness is analyzed in terms of surface roughening phenomena, and it is predicted that the values of growth and roughening exponent are 0.19 and 0.33, respectively, which is close to Kardar-Parisi-Zhang (KPZ) model. Furthermore, temporal evolution of surface chemistry, specifically surface hydroxyls and fluorine groups, are monitored. Surface density of fluorine moieties is 2.5 times higher than hydroxyl groups implying that the surface is well fluorinated during vapor etching.

2:30 PM

#### (GOMD-S1-089-2022) Transience of Mechanical Relaxation in Metallic Glass

L. Zella<sup>\*1</sup>; J. Moon<sup>2</sup>; T. Egami<sup>1</sup>

1. University of Tennessee, Materials Science and Engineering, USA
2. Oak Ridge National Lab, Materials Science and Technology Division, USA

Sinusoidal mechanical perturbation has been used to study the relaxation processes of glass at  $\sim 0.8T_g$  which is the region of  $\beta$ -relaxation. Studying relaxations at this temperature is important for the fundamental understanding of mechanical properties, such as ductility, brittleness and deformation. Previous works have analyzed how  $\beta$ -relaxation is modulated by defects defined by low density regions and to the amount of string-like motion. Our goal is to determine if other groups of atoms besides string-like motion cause relaxation and the importance of defects on the relaxation process by calculating atomic level mechanical loss. Using dynamic mechanical spectroscopy (DMS) in molecular dynamics (MD) simulation, we studied mechanical loss at  $\sim 0.8T_g$  in a prototypical  $\text{Cu}_{64.5}\text{Zr}_{35.5}$  metallic glass. Decomposition of system stress into individual atomic level stress enables identifying the groups of atoms responsible for mechanical loss. We determine that transient groups of atoms are causing the mechanical loss and find no direct relations for these atoms to local defects such as density defects. \*This work was supported by the U.S. Department of Energy (DOE), Office of Science, Office of Basic Energy Sciences, Materials and Science and Engineering Division.



2:50 PM

**(GOMD-S1-090-2022) Theoretical estimation of dielectric loss of oxide glasses using non-equilibrium molecular dynamics simulations (Invited)**S. Urata\*<sup>1</sup>; H. Hijjya<sup>1</sup>; K. Niwano<sup>1</sup>; J. Matsui<sup>2</sup>

1. AGC Inc., Japan
2. Kyushu University, Japan

To theoretically explore amorphous materials with a sufficiently low dielectric loss, which are essential for next-generation communication devices, the applicability of a non-equilibrium molecular dynamics simulation employing an external alternating electric field was examined using alkaline silicate glass models. In this method, the dielectric loss is directly evaluated as the phase shift of the dipole moment from the applied electric field. This method enabled us to evaluate the dielectric loss in a wide frequency range from 1 GHz to 10 THz. It was observed that the dielectric loss reaches its maximum at a few THz. The simulation method was found to qualitatively reproduce the effects of alkaline content and alkaline type on the dielectric loss. Furthermore, it reasonably reproduced the effect of mixed alkalines on the dielectric loss, which was observed in our experiments on sodium and/or potassium silicate glasses. Alkaline mixing was thus found to reduce the dielectric loss.

**S4: Glass Technology and Cross-Cutting Topics****3D Printing of Glass**

Room: Columbia (Second floor)

Session Chair: Laurent Gallais, Institut Fresnel

1:20 PM

**(GOMD-S4-026-2022) 3D Printing of Glass Imaging Optics with High Precision using a Liquid Silica Resin (Invited)**P. Ye<sup>2</sup>; Z. Hong<sup>3</sup>; R. Liang<sup>3</sup>; D. A. Loy\*<sup>1</sup>

1. The University of Arizona, Materials Science and Engineering, USA
2. The University of Arizona, Chemistry and Biochemistry, USA
3. The University of Arizona, Wyatt College of Optical Sciences, USA

3D Printing of optics has gained significant attention in the optical industry, but most of the research have been focused on organic polymers. In contrast, 3D printing inorganic glass has been achieved by filament, laser sintering, and vat photopolymerization methods, but burning out organics and sintering during densification gives rise to shrinkage, surface distortions, and limited quality. In order to attain optical quality suitable for micro-optics suitable for imaging, we developed a solvent-free, liquid silica resin (LSR) with minimal organics to achieve higher curing speed, better mechanical properties, lower thermal treatment temperature with no sintering required, reduced shrinkage, and, ultimately, glass optics with good surface quality. A two-photon polymerization process was utilized to print lenses from the LSR with flat, spherical, aspherical, freeform, and discontinuous surfaces with good surface shape and quality for imaging applications. Optical systems (e.g. micro-objective and micro-spectrometer) with multiple optical elements have also been printed and evaluated for imaging applications. Most importantly, we have also fabricated the micro-sized Alvarez lens pairs with moveable components. This study has paved the path for low-cost fabrication of complex glass optical systems for imaging applications.

1:50 PM

**(GOMD-S4-027-2022) 3D Printed Silica with Nanoscale Resolution (Invited)**J. Lou\*<sup>1</sup>

1. Rice University, USA

Fabricating inorganic materials with designed three-dimensional nanostructures is an exciting yet challenging area of research and industrial application. In this work, we develop an approach to 3D print high quality nanostructures of silica with sub-200 nm resolution and with flexible capability of rare earth element doping. The printed SiO<sub>2</sub> can be either amorphous glass or polycrystalline cristobalite controlled by the sintering process. The 3D printed nanostructures demonstrate attractive optical properties. For instance, the fabricated microtoroid optical resonators can reach quality factors (Q) over 10<sup>4</sup>. Moreover, importantly for optical applications, doping and co-doping of rare earth salts such as Er<sup>3+</sup>, Tm<sup>3+</sup>, Yb<sup>3+</sup>, Eu<sup>3+</sup> and Nd<sup>3+</sup> can be directly implemented in the printed SiO<sub>2</sub> structures, showing strong photoluminescence at the desired wavelengths. This technique shows the potential for building integrated microphotonics with silica via 3D printing.

2:20 PM

**(GOMD-S4-028-2022) Laser printing of fused silica parts based on multiphoton polymerization of photocurable nanosilica dispersions (Invited)**L. Gallais\*<sup>1</sup>; T. Doualle<sup>1</sup>; J. André<sup>2</sup>

1. Institut Fresnel, France
2. Laboratoire Réactions et Génie des Procédés, France

Different approaches have been developed or are under study to print three-dimensional glass structures. In this talk, we report on our recent progress in the development of a laser technique for 3D printing. It relies on multi-photon induced polymerization of photocurable nanosilica dispersions for the production of complex 3D silica parts. The technique is based on a focused, intense, laser beam that is used to polymerize a transparent resin at the wavelength of the laser beam through non-linear absorption processes. Thus, the object is created directly in the volume, avoiding addition of successive layers, overcoming the limitation of layer-by-layer process. Specific mixtures of resin with high viscosities loaded with soluble additives, mineral charges and nanoparticles with transparent properties, are used in order to avoid deformations during the construction process, strengthen the mechanical properties of the 3D objects and enable the production of mineral glasses with consecutive debinding and sintering processes. In its present development the process enables the production of centimetric silica parts with bulk silica density, that are intended to be used as optical components.

2:50 PM

**(GOMD-S4-029-2022) Optimisation of Powder Based Laser Additive Manufacturing of Soda Lime Silica Glass**F. Spirrett\*<sup>1</sup>; K. Datsiou<sup>1</sup>; R. Goodridge<sup>1</sup>; I. Ashcroft<sup>1</sup>; M. Magallanes<sup>2</sup>

1. University of Nottingham, United Kingdom
2. Glass Technology Services, United Kingdom

Laser additive manufacturing (AM) of glass powder onto substrates of the same composition is challenging due to various factors, such as high processing temperatures causing thermal shock of glass parts and substrates, and the low absorption of laser energy by glass powders with high transmittance in the near-IR range. This work demonstrates the potential to process soda lime silica glass onto substrates of the same composition by two AM methods; powder-fed directed energy deposition (DED), and selective laser melting (SLM). The successful fabrication of glass parts on glass substrates with good adhesion and limited thermal shock are presented. For powder-fed DED processing, parameters were optimised by energy density (ED) dependent on design feature and substrate thickness,

with 9.24 J/mm<sup>2</sup> used for curved features, and 12.6 J/mm<sup>2</sup> for straight features on 4 mm substrates, showing glass powder consolidation, adhesion of deposits to substrates, and little evidence of thermal shock. For SLM, optimisation of process parameters, such as energy density, scan strategy, and set-up, allowed fabrication of complex glass parts on glass substrates. This work demonstrates the potential to process glass powder onto glass substrates, allowing consideration of these techniques for industrial applications such as high-value glassware customisation, and fabrication of bespoke glass continuous flow reactors.

### 3:30 PM

#### (GOMD-S4-030-2022) Highly efficient, thermally robust and 3D printable green-emitting phosphor-in-glass composites

L. Qi<sup>\*1</sup>

1. Zhejiang University, China

High-power green solid-state light sources are essential to wide-color-gamut displays and high-color-rendering white lightings. However, traditional light-emitting diodes (LEDs) and laser diodes (LDs) suffer from the so-called “green gap”. Here, we report a highly efficient and thermally robust green color converter with Lu<sub>3</sub>Al<sub>5</sub>O<sub>12</sub>:Ce<sup>3+</sup> (LuAG:Ce) embedded in silica glass. We find that the interfacial reaction between LuAG:Ce particles and silica glass during the pressureless sintering process is very limited with an interface of only 50 nm in thickness, which endows such phosphor-in-glass (PiG) converter with high internal quantum efficiency (95%) and superior chemical and thermal stabilities. As such, we demonstrate a high-performance laser-driven green light source with high luminous efficacy of radiation (> 220 lm W<sup>-1</sup>), high power density (> 10 W mm<sup>-2</sup>) and high luminous flux (> 1500 lm) using the as-prepared PiGs doped with high concentration (> 30 wt%) of LuAG:Ce as the color converter. Furthermore, the proposed synthetic method is compatible with 3D printing technique, opening up the rapid manufacturing and mass customization of all-inorganic color converters for high-power phosphor-converted LED and LD light sources.

### 3:50 PM

#### (GOMD-S4-031-2022) Additive manufacturing of chalcogenide glasses for mid-infrared applications (Invited)

J. Troles<sup>\*1</sup>; J. Carcreff<sup>1</sup>; F. Chevire<sup>1</sup>; R. Lebullenger<sup>1</sup>; A. Gautier<sup>1</sup>; R. Chahal<sup>2</sup>; L. Calvez<sup>3</sup>; C. Boussard-Pledel<sup>1</sup>; L. Brilland<sup>2</sup>; F. Charpentier<sup>3</sup>; H. Tariel<sup>2</sup>; Y. Guimond<sup>4</sup>; M. Rozé<sup>4</sup>; L. Szymczyk<sup>4</sup>; G. Renversez<sup>5</sup>

1. University of Rennes 1, France
2. SelenOptics, France
3. Diafir, France
4. Umicore IR Glass, France
5. Aix-Marseille Univ, Institut Fresnel, France

In recent years, a growing interest has settled for optical materials and fibers for the mid infrared (mid-IR) region. This interest originates from societal needs for health and environment for instance, and also from demand for defence applications. Indeed, the mid-IR spectral region contains the atmospheric transparent windows (3-5 μm) and (8-12 μm) where thermal imaging (military and civilian) can take place. In this context, we have investigated an alternative way for fabricating Mid-IR optical components such as preforms, optical fibers, sensors and lenses by using an original 3D printing process. In our work, the 3D-printing set-up has been specially designed for chalcogenide glasses. Especially, the feeding mechanism is customized for glass materials. By using this additive manufacturing method, preforms with complex designs can be fabricated in a single step within a couple of hours, with a high degree of repeatability and precision of the geometry. This original 3D printing method, opens the way to many applications involving chalcogenide fibers manufacturing but also many other chalcogenide glass optical components

Thursday, May 26, 2022

## Award Lectures

### Varshneya Glass Technology Lecture

Room: Constellation C/D (Second floor)

Session Chair: Gang Chen, Ohio University

#### 8:10 AM

#### (GOMD-AW-005-2022) From strong bioactive glasses to tough bio-inspired glass-ceramics: A journey towards damage-resistant materials

Q. Fu<sup>\*1</sup>

1. Corning Incorporated, USA

The quest for damage-resistant engineering materials for biomedical, structural and technical applications is driving the development of high-performance materials with exceptional mechanical properties. Bioactive glass, invented in 1960s, was initially targeted for soft tissue or non-loaded hard tissue regeneration. Despite its brittleness, recent advances in new glass compositions and processing techniques have demonstrated the potential to produce glass scaffolds with strength comparable to that of cortical bone, opening a new avenue for their applications in loaded large bone defects. On the other hand, glass-ceramics were born tough when discovered in 1950s. New improvements in this material family, inspired from natural biological and geological minerals, have made possible unique microstructures and phase assemblages. The resulting glass-ceramics have demonstrated superior damage-resistance due to their exceptional strength and toughness, enabling their applications beyond traditional consumer products.

## S2: Glass and Interactions with Its Environment: Fundamentals and Applications

### Surfaces and Coatings

Room: Constellation F (Second floor)

Session Chair: Matthew Linford, Stanford University

#### 9:20 AM

#### (GOMD-S2-050-2022) Non-uniform glass surface chemistry and its role in producing delaminated flakes in pharmaceutical containers (Invited)

R. Schaut<sup>\*1</sup>; S. A. Tietje<sup>1</sup>; D. Ragland<sup>1</sup>; D. Kramer<sup>2</sup>; E. Bakowska<sup>3</sup>

1. Corning Incorporated, S&T, Glass Research, USA
2. Corning Incorporated, Pharmaceutical Technologies, USA
3. Corning Incorporated, Characterization Sciences, USA

Delamination of pharmaceutical glass containers has been linked to non-uniform surface chemistry produced during the tube-to-container forming process. The degree to which the surface is chemically altered is influenced by the forming conditions and has direct impact on how rapidly the altered regions corrode to release flakes into solution. Here we will explore the influences of testing conditions upon the corrosion of delamination-prone containers and illustrate the role of the drug product on flake production. The glass composition-dependence of corrosion rate is highlighted as it relates to the production of delamination flakes during non-accelerated drug storage conditions. A complete view of the interface will be provided by characterizing the parent glass, altered surface, solution chemistry, and resulting defects. Comparisons will be made to containers with uniform surface chemistry which do not exhibit delamination.

9:50 AM

**(GOMD-S2-051-2022) Modification of Multicomponent Glass Surfaces with HF Vapors**N. J. Smith<sup>\*1</sup>; G. Agnello<sup>1</sup>; J. Banerjee<sup>1</sup>; H. Park<sup>1</sup>; R. Yongsunthon<sup>1</sup>; K. Adib<sup>1</sup>; A. Antony<sup>1</sup>

1. Corning Incorporated, USA

Glass surface modification is an area of perpetual interest for technical glass products in modern applications. Among the variety of techniques available to alter glass surface properties, one relatively unexplored area relates to treatments with reactive hydrofluoric acid (HF) vapors, ostensibly due to the significant health hazards posed by HF gas. This difficulty has limited detailed and rigorous studies of its interactions with multicomponent glass surfaces, with scarce understanding on how different HF gas concentrations or mixtures physically alter surface properties. Moreover, although such treatments are often referred to as “dry” etching since there is no bulk liquid involved, it is also known that water is, in fact, a very active participant in vapor-phase etching reaction(s) of HF with oxide glasses. To examine these effects more rigorously, we constructed a custom gas-flow reactor that allows us to safely expose glass samples to mixtures of HF and H<sub>2</sub>O vapors (independently-controlled), leveraging in-situ FTIR spectroscopy to monitor concentrations of gas-phase reactants and by-products. With focus on representative glasses used as display substrates, we report on measured etch rates based on two different methods (step-height, and inferred from FTIR data), as well as numerous observations of modified composition and topography that point the way to tailored surface properties.

10:10 AM

**(GOMD-S2-052-2022) Interfacial optical effects as revealed with scattering scanning near field optical microscopy (sSNOM) on acid leached soda lime silica (SLS) glass reveal limitations of plug-and-chug spectroscopy**A. L. Ogrinc<sup>\*1</sup>; Y. Zhou<sup>2</sup>; S. Hahn<sup>4</sup>; T. Gokus<sup>2</sup>; S. H. Kim<sup>1</sup>

1. Pennsylvania State University, Chemical Engineering, USA
2. neaspec, Germany
3. University of Illinois at Urbana-Champaign, USA
4. Samsung Electronics, Republic of Korea

Specular reflection infrared spectroscopy (SR-IR) has long been used to analyze the surfaces of silicate glasses, with the band at ~950 cm<sup>-1</sup> being correlated to the vibrational response of nonbridging oxygen species which are either Si-O<sup>-</sup> or Si-OH. This assignment was examined by comparing the vibrational spectra of two techniques that have different probe depths; SR-IR which has a probe depth of ~600 nm at ~1100 cm<sup>-1</sup>, and sSNOM which has a probe depth of ~20 nm. A ~140 nm thick Na-leached layer was created on SLS through treatment at pH 1 for 1 week at 90°C. After treatment, the signal in SR-IR at 950 cm<sup>-1</sup> was enhanced, which could imply an increase in the Si-OH concentration upon leaching of Na. However, the sSNOM analysis showed that the intensity at 950 cm<sup>-1</sup> actually decreased. A simulation with the optical constant obtained from sSNOM revealed that the increase of the 950 cm<sup>-1</sup> band in SR-IR is an artifact due to optical interferences. In fact, the Si-O bond length distributions obtained from molecular dynamics simulations suggested the vibrational mode involving Si-OH groups would not have absorption at ~950 cm<sup>-1</sup>. These results challenge the conventional assignment of the 950cm<sup>-1</sup> band in vibrational spectral analysis of silicate glass and a new interpretation scheme is proposed.

10:30 AM

**(GOMD-S2-053-2022) Non-destructive characterization of corroded glass surfaces (Invited)**T. Kaspar<sup>\*1</sup>

1. Pacific Northwest National Lab, Physical and Computational Sciences Directorate, USA

Exposure of glass to harsh chemical environments leads, over time, to corrosion of the glass surface. Dissolution of glass species into the environment, often accompanied by ingress of aqueous species into the surface region of the glass, results in “alteration” layers on the glass surface. Characterization of these layers in laboratory-based accelerated corrosion testing is key to predicting the behavior of nuclear wasteform glass over geologic timescales. In recent studies, modern materials science tools have been utilized to characterize these alteration layers after corrosion. Here I will present a study treating the alteration layer as a thin film and characterizing it with non-destructive spectroscopic ellipsometry (SE). The information we can gain from SE is compared to the non-destructive techniques small-angle x-ray scattering (SAXS) and positron annihilation spectroscopy, and to the alteration layer properties determined by traditional characterization techniques (scanning electron microscopy, aqueous solution analysis). Our results show that corroded alteration layers are complex but (in many cases) tractable “thin films”, and meaningful information on their thickness, morphology, and porosity can be extracted from SE measurements.

11:00 AM

**(GOMD-S2-054-2022) Glass surface under stress -- what do we know about the stress effect on mechanical properties?**S. H. Kim<sup>\*1</sup>; H. Liu<sup>1</sup>

1. Pennsylvania State University, Chemical Engineering &amp; Materials Science, USA

As a means to elucidate the mechanical stress effect on the durability of soda lime silicate (SLS) float glass, a thin glass plate under flexural stress was investigated. A lab-built four-point bending rig was employed to create compressive or tensile stress (around 40 MPa) on the air-side surface of SLS glass. The elastic and plastic responses of the SLS surface to nanoindentation were significantly altered under the flexural stress conditions even though the magnitude of the flexural stress was less than 0.7% of the applied indentation stress. Compared to the stress-free surface, the resistance to mechanochemical wear at 90% relative humidity deteriorated under the compressive stress condition, while it just became more scattered under the tensile stress condition. Even though the applied flexural stress was very small, its impact on chemical and structural properties could be surprisingly large, could not be explained with simple force balance or stress corrosion arguments. Combining all results in this study and previously published works suggested that the changes observed in nanoindentation and mechanochemical wear behaviors may be associated with the strain in the Si-O bonds of the silicate network.

11:20 AM

**(GOMD-S2-055-2022) Chemical and physical properties of aluminoborosilicate glass surfaces treated with alkaline solutions of variable strength and/or component ratio**G. Agnello<sup>\*1</sup>; N. J. Smith<sup>1</sup>; J. Banerjee<sup>1</sup>; M. Bell<sup>1</sup>; C. V. Cushman<sup>1</sup>; A. Antony<sup>1</sup>; H. Park<sup>1</sup>

1. Corning Incorporated, USA

Cleaning processes for glasses can and do include both acidic and basic components, where the choice of which type and/or combination depends largely on the intended application. If we think of these two classes of treatments in terms of pH, the interactions between a glass surface and a pH<7 media will be different than interactions involving high pH (~10-14) reactants. Therefore, we should reasonably expect that the intrinsic properties of surfaces



treated with alkaline based chemistries to be different as well. In a previous talk (GOMD/PACRIM 2021), we reported on experiments which probed flat glass surface properties resulting from treatment with different types of acidic solutions, namely pure HF of variable concentration and HF:HCl of variable component ratio. In these experiments, the topmost 0.1-3nm of the surfaces were assessed for physical and chemical changes using different surface-sensitive techniques including contact angle measurements (surface free energy), zeta potential, atomic force microscopy (AFM) and Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS). Here, we present results from complementary experiments on glasses treated with alkaline formulations (NH<sub>4</sub>OH:H<sub>2</sub>O<sub>2</sub>:H<sub>2</sub>O [commonly known as SC1], KOH and commercially available surfactant-based detergent) of variable concentration and/or component ratio.

### 11:40 AM

#### (GOMD-S2-056-2022) Photothermal AFM-IR Analysis of High Extinction Coefficient Materials: A Case Study with Silica and Silicate Glasses

Y. Lin<sup>\*1</sup>; H. He<sup>2</sup>; H. Kaya<sup>3</sup>; H. Liu<sup>4</sup>; D. Ngo<sup>1</sup>; N. J. Smith<sup>4</sup>; J. Banerjee<sup>4</sup>; A. Borhan<sup>1</sup>; S. H. Kim<sup>1</sup>

1. Pennsylvania State University, Chemical Engineering, USA
2. Southwest University of Science and Technology, China
3. Pennsylvania State University, USA
4. Corning Incorporated, USA

Photothermal atomic force microscopy coupled with infrared spectroscopy (AFM-IR) brings significant value as a spatially-resolved surface analysis technique for disordered oxide materials such as glasses, but additional development and fundamental understanding of governing principles is needed to interpret AFM-IR spectra, given the existing theory fails to describe the materials with high extinction coefficients for IR absorption. We propose a theoretical calculation model of a transient temperature profile inside the IR-absorbing material considering IR refraction at the interface as well as IR adsorption and heat transfer inside the sample. This calculation aligns well with the experimental spectra and explains the differences in peak positions and amplitudes of AFM-IR spectra from those of specular reflectance and extinction coefficient spectra. It also addresses the information depth of the AFM-IR characterization of bulk materials. AFM-IR applied to silica and silicate glass surfaces has demonstrated the capability of characterizing sub-surface structural changes and surface heterogeneity due to mechanical stresses from physical contacts as well as chemical alterations manifested in surface layers through aqueous corrosion.

### 12:00 PM

#### (GOMD-S2-057-2022) Effect of Vickers Indentation Flaws on Chemical Strengthening of SLS Glass

C. Budziszewski<sup>\*1</sup>; W. LaCourse<sup>1</sup>

1. Alfred University, Inamori School of Engineering, USA

Float glass (air side) with Vickers indentation flaw depths of up to 85 microns were strengthened by a K<sup>+</sup> for Na<sup>+</sup> ion-exchange process. Strengthening occurred in glass with all crack lengths, but the effect of ion-exchange time and pre-exchange stress relaxation depended on crack size. Glass with crack lengths greater than about 40 microns initially strengthened (~ 1 hour) followed by a slow decrease in MOR before again strengthening. Samples with cracks less than 40 microns exhibited normal behavior, with an initial rapid strengthening followed by continued strengthening at slower rates. 3 mechanisms that can cause or contribute to the cause of the observed behavior will be discussed. All assume “accessible” cracks with K<sup>+</sup> reaching the crack tips via capillary motion and surface diffusion, followed by contamination of the liquid by Na<sup>+</sup> and Ca<sup>++</sup> and by crack closure at the surface.

### 12:20 PM

#### (GOMD-S2-058-2022) A Tag-and-Count Approach for Quantifying Surface Silanol Densities on Fused Silica Based on Atomic Layer Deposition and High-Sensitivity Low-Energy Ion Scattering

T. Gholian Avval<sup>1</sup>; S. Prusa<sup>3</sup>; C. V. Cushman<sup>2</sup>; G. Hodges<sup>1</sup>; S. Fearn<sup>4</sup>; J. Cechal<sup>5</sup>; T. Sikola<sup>3</sup>; H. Brongersma<sup>6</sup>; M. R. Linford<sup>\*1</sup>

1. Brigham Young University, Department of Chemistry and Biochemistry, USA
2. Corning Incorporated, Science & Technology Division, USA
3. Brno University of Technology, Institute of Physical Engineering, Czechia
4. Imperial College of London, Department of Materials, United Kingdom
5. Brno University of Technology, CEITEC, Czechia
6. Eindhoven University of Technology, Department of Applied Physics, Netherlands

Surface hydroxyls, e.g., silanols (SiOH), are among the most important and reactive sites on glass surfaces, playing a critical role in glass surface modification and reactivity. Here we present a tag-and-count approach for determining surface silanol density, which consists of tagging surface silanols with Zn via atomic layer deposition (ALD) followed by detecting Zn atoms by low energy ion scattering (LEIS). Here, shards of fused silica were hydroxylated with aqueous HF and then heated to 200, 500, 700, or 900 °C. These treatments increasingly condense and remove surface silanols to tune the surface silanol density. The samples then underwent one ALD cycle of dimethylzinc (DMZ) or diethylzinc (DEZ) and water. The coverage of Zn on the surfaces was then determined using LEIS. Surface cleaning/preparation immediately before LEIS, which included atomic oxygen treatment and annealing, played a critical role in these efforts. As expected, fused silica surfaces heated to lower temperatures consistently showed higher Zn coverages. Surfaces treated with DMZ showed slightly higher Zn signals by LEIS, presumably because of its lower steric hindrance compared to DEZ. However, this difference disappeared in the case of the surfaces treated at 900 °C where the silanol concentration should be the lowest.

## S3: Optical and Electronic Materials and Devices: Fundamentals and Applications

### Optical Fibers and Waveguides

Room: Frederick (Second floor)

Session Chair: Jiawei Luo, OFS Laboratories

### 9:20 AM

#### (GOMD-S3-035-2022) Engineering the characteristics of nanoparticles in preforms and optical fibers (Invited)

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In order to offer new application opportunities, it was proposed twenty years ago to insert nanoparticles into the core of optical fibers. The first targeted application concerned the engineering of luminescence properties to develop new lasers and amplifiers. More recently, such fibers have demonstrated great interest as sensors (stress, temperature, chemical environment, etc.). The success of



these applications relies on our ability to control the characteristics of nanoparticles. In the case of lasers/amplifiers, small nanoparticles are usually sought to limit losses induced by light scattering. On the contrary, sensors exploit light scattering and therefore require large particles. During this presentation, we will discuss the control of particle properties in the preform and the fiber. As known in bulk glass, the chemical element and its concentration make it possible to control the average size of the particles in the preform. However, we will take this opportunity to show that the smallest particles are not the most relevant for luminescence properties. Finally, the characteristics (size and shape) of the particles in the fibers can be determined from the drawing conditions or heat treatments applied a posteriori. All these approaches demonstrate the ability to tune the shape and size of the nanoparticles in fibers thanks to appropriate heat treatment.

**9:50 AM**

**(GOMD-S3-036-2022) Challenges and opportunities of multi-material optical fibers (Invited)**

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Fiber-integrated photonics is at the heart of the development of novel applications in advanced optical probes for health care and bioengineering, robotics, sensing, and smart textiles. Advances in fluid dynamic based processes is now allowing the tailoring of complex architectures of optical glasses, polymers and metals over thin-films and fiber substrates. In particular, the thermal drawing process used to make optical fibers has known a series of breakthroughs in recent years that have expanded the range of materials and architectures that can be engineered within flexible and stretchable optical fibers. In this talk, I will review important novel aspects for the materials choice and the physical phenomena at play in the thermal drawing process. I will explain how we can exploit these novel understandings to make advanced optical fibers with new functionalities. I will in particular discuss different sensing and energy harvesting schemes based on multi-material optical fibers integrating thermoplastic elastomers and liquid metal domains. I will also present how advanced biodegradable and even food-grade optical fibers can be fabricated and how this opens novel opportunities for fiber photonics.

**10:20 AM**

**(GOMD-S3-038-2022) Elaboration and loss optimization of niobium rich borophosphate optical glass fibers**

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Here we explore the manufacturing of BPN glasses into fibers with optical quality. Glass preforms with different Niobium oxide concentrations were synthesized and thermally drawn. Viscosity measurements performed in the softening point range show that the optical fiber drawing temperature gradually increases with the amount of niobium oxide. X-ray diffraction and Raman structural analysis performed post-drawing demonstrate that the BPN glass with 39% Nb<sub>2</sub>O<sub>5</sub> represents the upper limit for fiber drawing under oxygen. Subsequently, preform quenching protocol was optimized to mitigate the density fluctuations within the glass matrix related to convection flows and compare with the conventional cast-in-mold method. Shadowscopy imaging highlights the improvement in the optical quality of the glasses produced following this new protocol. This observation is confirmed by cut back loss measurements which show a decreasing in the attenuation from 6.04 dB/m to 3.19 dB/m between the two methods. We believe the manufacturing of niobium rich borophosphate fibers with improved optical quality paves the way toward their potential use as near-IR highly nonlinear waveguide devices.

**10:40 AM**

**(GOMD-S3-039-2022) Multifunctional ferromagnetic fiber robots for navigation, imaging, and optical modulation in biomedical applications**

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Small-scale continuum robots capable of remote active steering and navigation offer great opportunities for biomedical applications. However, due to the miniaturization and fabrication challenges, current continuum robots are often limited to millimeter or centimeter scales and are hard to be integrated with other functionalities. Here, we present a sub-millimeter ferromagnetic fiber robotic platform for integrating navigation, imaging, and optical modulation fabricated via a thermal drawing process. By using tortuous blood vascular phantom and agarose gel brain phantom, we demonstrate the capability of navigating through minimally invasive cardiovascular surgery and neural probe insertion based on magnetic actuation. Additionally, we experimentally show that the fiber can be potentially used for imaging and laser delivery with embedded waveguides. Furthermore, we demonstrate the ability of our fiber robots capturing brain activities with a single unit resolution and optical modulation of brain activities using in vivo mouse models. Given their compact form factor and multifunctionality, our ferromagnetic fiber robots have potentials to get access to and provide treatment for previously inaccessible lesions, thereby improving surgical outcomes.

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